Supporting Information for:

Synthesis, Structure, and Activity of Enhanced Initiators for Olefin Metathesis

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Experimental Section

(H_2IMes)[(*p*-$CF_3C_6H_4)_3$P]$(Cl)_2$Ru=CHPh (6). Complex **12** (200 mg, 0.275 mmol) and (*p*-$CF_3C_6H_4)_3$P (140 mg, 0.300 mmol) were combined in benzene (2 mL), and the resulting solution was stirred for 10 minutes. The solution was frozen using a dry-ice/acetone bath and the solvent was removed under vacuum. Benzene (1 mL) was added to the resulting brown residue. The solution was again frozen and the solvent was removed under vacuum. This cycle was repeated a third time, then the resulting brown residue was washed with 3 x 3 mL pentane and dried under vacuum at room temperature. Complex **6** was obtained as a pink powder (145 mg, 51% yield). $^{31}P\{^1H\}$ NMR (CD_2Cl_2): δ 40.20 (s). ^{19}F NMR (CD_2Cl_2): δ –63.17 (s). ^1H NMR (CD_2Cl_2): δ 19.11 (s, 1H, Ru=C*H*Ph), 7.37 (d, 6H, C*H* (*p*-$CF_3C_6H_4)_3$P, J_{HH} = 7 Hz), 7.32 (d, 2H, ortho C*H*, J_{HH} = 7 Hz), 7.29 (t, 1H, para C*H*, J_{HH} = 7 Hz), 7.04 (t, 8H, Mes C*H* and C*H* (*p*-$CF_3C_6H_4)_3$P, J_{HH} = 9 Hz), 6.77 (t, 2H, meta C*H*, J_{HH} = 8 Hz), 6.36 (s, 2H, Mes C*H*), 4.04 (m, 4H, CH_2CH_2), 2.61 (s, 6H, ortho CH_3), 2.44 (s, 3H, para CH_3), 2.22 (s, 6H, ortho CH_3), 1.93 (s, 3H, para CH_3). $^{13}C\{^1H\}$ NMR (CD_2Cl_2): δ 308.18-306.94 (multiple peaks, Ru=*C*HPh), 217.03 (d, Ru-*C*$(N)_2$, J_{CP} = 94 Hz), 151.60 (m), 139.82, 139.18, 138.77 (d), 137.44, 137.22, 135.46, 138.48 (t), 134.53, 134.23, 132.12 (q), 130.60, 130.51, 130.37, 130.29, 130.20 (d), 129.68 (d), 128.15, 127.99, 127.69 (d), 125.52, 125.13 (m), 123.26, 121.19, 52.60 (m), 51.81 (m), 21.24 (qu), 20.48 (q), 19.90, 18.69 (q). Anal. Calcd for $C_{49}H_{44}N_2F_9Cl_2PRu$: C, 56.87; H, 4.29; N, 2.71. Found: C, 56.99; H, 4.48; N, 2.60.

(H_2IMes)[(p-ClC_6H_4)$_3$P]$(Cl)_2$Ru=CHPh (7). Complex **12** (200 mg, 0.275 mmol) and (p-ClC_6H_4)$_3$P (120 mg, 0.328 mmol) were combined in benzene (2 mL) and stirred for 10 minutes. The solvent was removed under vacuum, and the resulting brown residue was washed with 5 x 5 mL pentane and dried under vacuum. Complex **7** was obtained as a pink powder (180 mg, 70% yield). $^{31}P\{^1H\}$ NMR (C_6D_6): δ 37.10 (s). ^1H NMR (C_6D_6): δ 19.50 (s, 1H, Ru=C*H*Ph), 7.63 (d, 2H, ortho C*H*, J_{HH} = 8 Hz), 7.16-6.69 (multiple peaks, 17H, (p-ClC_6H_4)$_3$P, para C*H*, meta C*H*, and Mes C*H*), 6.30 (s, 2H, Mes C*H*), 3.31 (m, 4H, CH_2CH_2), 2.72 (s, 6H, ortho CH_3), 2.36 (s, 6H, ortho CH_3), 2.34 (s, 3H, para CH_3), 1.89 (s, 3H, para CH_3). $^{13}C\{^1H\}$ NMR (C_6D_6): δ 306.08 (m, Ru=*C*HPh), 218.53 (d, Ru-*C*$(N)_2$, J_{CP} = 93 Hz), 151.70 (d, J_{CP} = 3 Hz), 139.77, 138.94, 138.35, 137.70, 137.68 (d, J_{CP} = 2 Hz), 136.21, 135.67, 131.08, 130.46, 129.86, 129.75, 129.62, 129.32, 128.68, 128.03, 52.04 (d, J_{CP} = 4 Hz), 51.38 (d, J_{CP} = 2 Hz), 21.68, 21.31, 21.94, 19.06. Anal. Calcd for $C_{46}H_{44}N_2Cl_5PRu$: C, 59.14; H, 4.75; N, 3.00. Found: C, 58.77; H, 4.63; N, 3.22.

(H_2IMes)(PPh_3)$(Cl)_2$Ru=CHPh (9). Complex **12** (1.85 g, 2.55 mmol) and PPh_3 (750 mg, 2.86 mmol) were combined in benzene (10 mL) and stirred for 20 minutes. The solvent was removed under vacuum, and the resulting brown residue was washed with 5 x 25 mL pentane and dried under vacuum. Complex **9** was obtained as a brownish-orange powder (1.55 mg, 73% yield). $^{31}P\{^1H\}$ NMR (C_6D_6): δ 37.7 (s). ^1H NMR (C_7D_8): δ 19.60 (s, 1H, Ru=C*H*Ph), 7.70 (d, 2H, ortho C*H*, J_{HH} = 8 Hz), 7.29-6.71 (multiple peaks, 20H, P*Ph*$_3$, para C*H*, meta C*H*, and Mes C*H*), 6.27 (s, 2H, Mes C*H*), 3.39 (m, 4H, CH_2CH_2), 2.74 (s, 6H, ortho CH_3), 2.34 (s, 6H, ortho CH_3), 2.23 (s, 3H, para CH_3), 1.91 (s, 3H, para CH_3). $^{13}C\{^1H\}$ (C_6D_6) δ 305.34 (m, Ru=*C*HPh), 219.57 (d, Ru-*C*$(N)_2$, J_{CP} = 92 Hz), 151.69 (d, J_{CP} = 4 Hz), 139.68, 138.35, 138.10, 138.97, 137.78, 135.89, 135.21, 135.13, 131.96, 131.65, 131.36, 130.47, 129.83, 129.59 (d, J_{CP} = 2 Hz), 129.15, 128.92, 128.68, 128.00, 52.11 (d, J_{CP} = 4 Hz), 51.44 (d, J_{CP} = 2 Hz), 21.67, 21.35, 21.04,

19.21. HRMS (FAB) Calcd: 830.1897 (M^+). Found: 830.1894. Anal. Calcd for $C_{46}H_{47}N_2Cl_2PRu$: C, 66.50; H, 5.70; N, 3.37. Found: C, 66.82; H, 5.76; N, 3.29.

(H_2IMes)[(p-MeOC_6H_4)$_3$P](Cl)$_2$Ru=CHPh (11). Complex **12** (200 mg, 0.275 mmol) and (p-MeOC_6H_4)$_3$P (105 mg, 0.298 mmol) were combined in benzene (2 mL) and stirred for 10 minutes. The solvent was removed under vacuum, and the resulting brown residue was washed with 5 x 3 mL pentane and dried under vacuum. Complex **11** was obtained as a pink powder (160 mg, 63% yield). $^{31}P\{^1H\}$ NMR (CD_2Cl_2): δ 35.52 (s). ^1H NMR (CD_2Cl_2): δ 19.16 (s, 1H, Ru=C*H*Ph), 7.41 (d, 2H, ortho C*H*, J_{HH} = 5 Hz), 7.36 (m, 2H, meta C*H*), 7.29 (t, 1H, para C*H*, J_{HH} = 5 Hz), 7.05 (s, 2H, Mes C*H*), 6.81 (m, 6H, C*H* (p-MeOC_6H_4)$_3$P), 6.61 (m, 6H, C*H* (p-MeOC_6H_4)$_3$P), 6.36 (s, 2H Mes C*H*), 4.00 (m, 4H, CH_2CH_2), 3.75 (s, 9H, OCH_3), 2.63 (s, 6H, ortho CH_3), 2.44 (s, 6H, ortho CH_3), 2.23 (s, 3H, para CH_3), 1.96 (s, 3H, para CH_3). $^{13}C\{^1H\}$ NMR (CD_2Cl_2): δ 303.85 (d, Ru=*C*HPh, J_{CP} = 9 Hz), 219.34 (d, Ru-*C*(N)$_2$, J_{CP} = 91 Hz), 161.14 (d, J_{CP} = 2 Hz), 151.10 (d, J_{CP} = 4 Hz), 139.61, 138.71, 138.34, 137.65, 137.40, 135.85 (d, J_{CP} = 13 Hz), 130.87, 130.08, 129.60, 129.24, 128.85, 127.81, 122.97, 122.62, 113.60 (d, J_{CP} = 10 Hz), 55.66, 52.56 (d, J_{CP} = 4 Hz), 51.78 (d, J_{CP} = 3 Hz), 21.65, 21.18, 20.48, 18.77. Anal. Calcd for $C_{49}H_{53}N_2Cl_2O_3PRu$: C, 63.91; H, 5.80; N, 3.04. Found: C, 64.49; H, 5.84; N, 3.03.

Table S1. Rate Constants for and T_1 values for Phosphine Exchange in **6–11**.

Complex	k_{obs}/s^{-1}	eq PR_3	T (K)	T_{1F}/s	T_{1C}/s
6	3.9 ± 0.2	1.5 eq	323	9.1	3.0
	10 ± 1	1.5 eq	333	11.6	3.1
	23 ± 2	1.5 eq	343	9.0	3.3
	48 ± 2	1.5 eq	353	10.2	3.2
	47.6 ± 0.9	5 eq	353	9.5	3.0
7	1.44 ± 0.08	1.5 eq	323	9.2	5.0
	2.8 ± 0.1	1.5 eq	333	10.7	7.1
	7.0 ± 0.3	1.5 eq	343	9.9	3.1
	17.9 ± 0.4	1.5 eq	353	10.2	3.6
	17.7 ± 0.5	5 eq	353	10.7	3.0
8	0.5 ± 0.1	1.5 eq	323	11.5	4.0
	1.0 ± 0.1	1.5 eq	333	11.0	4.2
	3.1 ± 0.5	1.5 eq	343	9.9	3.7
	8.5 ± 0.2	1.5 eq	353	9.9	4.0
	8.9 ± 0.3	5 eq	353	10.3	4.2
9	0.049 ± 0.008	1.5 eq	303	17.8	4.1
	0.138 ± 0.005	1.5 eq	313	18.5	4.2
	0.420 ± 0.008	1.5 eq	323	20.0	4.5
	1.22 ± 0.02	1.5 eq	333	16.7	5.5
	0.11 ± 0.05	5 eq	313	20.0	3.5
	0.14 ± 0.04	10 eq	313	19.2	3.3
10	0.8 ± 0.1	1.5 eq	333	13.2	3.8
	2.1 ± 0.1	1.5 eq	343	14.1	2.7
	4.1 ± 0.2	1.5 eq	353	14.0	3.6
	11.4 ± 0.3	1.5 eq	363	13.3	3.3
	11.1 ± 0.3	5 eq	363	12.6	3.0
11	0.15 ± 0.02	1.5 eq	323	11.5	1.7
	0.29 ± 0.04	1.5 eq	333	10.7	2.2
	0.80 ± 0.07	1.5 eq	343	11.2	3.0
	1.8 ± 0.1	1.5 eq	353	11.0	3.3
	1.8 ± 0.1	5 eq	353	14.0	2.8

Table S2. T_1 Analysis for complexes **6-11** in C_7D_8 solution.

Complex	T_1 (s^{-1})
P(*p*-$CF_3C_6H_4$)$_3$	12 ± 1
P(*p*-ClC_6H_4)$_3$	11.7 ± 0.9
P(*p*-FC_6H_4)$_3$	11.5 ± 0.8
P(C_6H_5)$_3$	23.7 ± 0.6
P(*p*-$CH_3C_6H_4$)$_3$	13 ± 2
P(*p*-$CH_3OC_6H_4$)$_3$	13.2 ± 0.9
6	1.8 ± 0.9
7	2.3 ± 0.8
8	3.0 ± 0.5
9	3.5 ± 0.2
10	3.0 ± 0.4
11	3.2 ± 0.8

Table S3. Activation parameters for complexes **4**, **6-11,** and **14**[a,b]

Catalyst	$\Delta H^{\ddagger}$ (kcal/mol^{-1})	$\Delta S^{\ddagger}$ (cal/mol ^{o}K)	$\Delta G^{\ddagger}$ (298 K) (kcal/mol^{-1})
4	27.6 ± 0.5	5 ± 2	26.1 ± 0.5
6	18.3 ± 0.6	1 ± 1	18.1 ± 0.6
7	19.9 ± 0.4	3 ± 1	18.9 ± 0.4
8	23 ± 1	12 ± 3	20 ± 1
9	21.9 ± 0.4	7 ± 1	19.7 ± 0.4
10	20.8 ± 0.7	3 ± 2	19.9 ± 0.7
11	19 ± 1	-5 ± 4	20 ± 1
14	19.9 ± 0.5	1 ± 2	19.6 ± 0.5

[a] The activation parameters were determined using a nonlinear least-squares analysis using Origin. [b] Error was determined taking the covariance of $\Delta H^{\ddagger}$ and $\Delta S^{\ddagger}$ into consideration.

Rate Equation Used for Determination of k_{-1}/k_2:

$$1/k_{obs} = k_{-1}[PR_3]/k_1k_2[olefin] + 1/k_1$$

This was derived from the Steady-State rate equation:

$$\text{Rate} = k_1k_2[Ru][PR_3][olefin] / (k_{-1}[PR_3] + k_2[olefin])$$

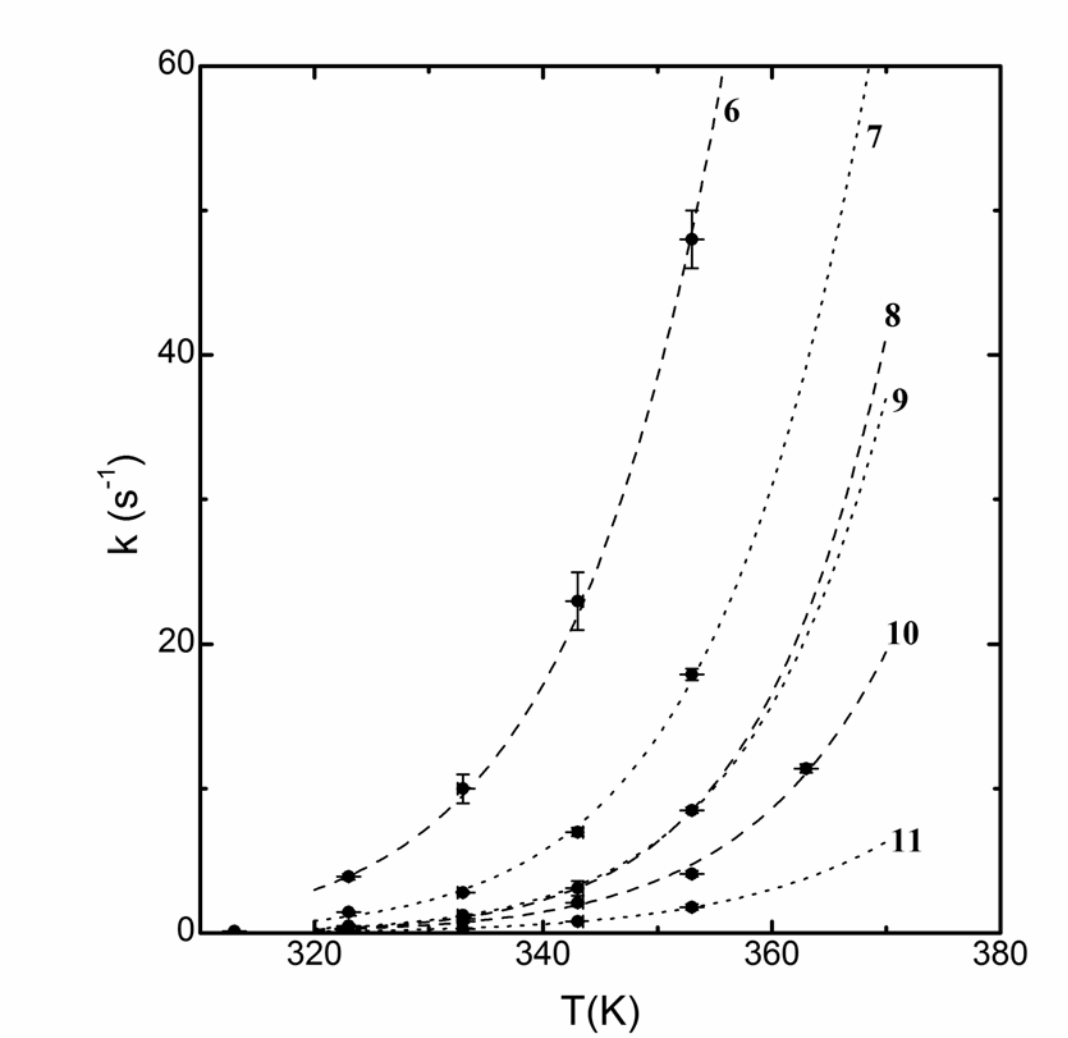
$$k_{obs} = k_1k_2[PR_3][olefin] / (k_{-1}[PR_3] + k_2[olefin])$$

Table S4. Values of k_1 from $1/k_{obs}$ versus $[PR_3]/[olefin]$.

Complex	k_1 $(s^{-1})^a$	k_1 (predicted) $(s^{-1})^b$
6	0.35	0.34
7	0.011	0.11
8	0.006	0.026
9	0.013	0.025
10	0.0086	0.020
11	0.0034	0.011

[a] k_1 values are from 1/intercept. [b]] k_1 values determined from Eyring plots from magnetization transfer experiments.

Figure S1. Nonlinear least-squares analysis of magnetization transfer data for **6-11**.



Kinetic data were fit to the Arrhenius equation using the non-linear least squares Levenberg-Marquardt (LM) regression analysis provided in the Microcal Origin Professional 7.0 software package. The statistical errors in the experimental rate constants were used as weighting factors for χ^2 minimization (using the 'instrumental' error analysis function within Origin). All non-linear fits provided robust fits with $r^2 > 0.987$ in all cases.

Figure S2. $1/k_{obs}$ vs. [P(*p*-$CF_3C_6H_4)_3$]/[olefin] for Catalyst **6**

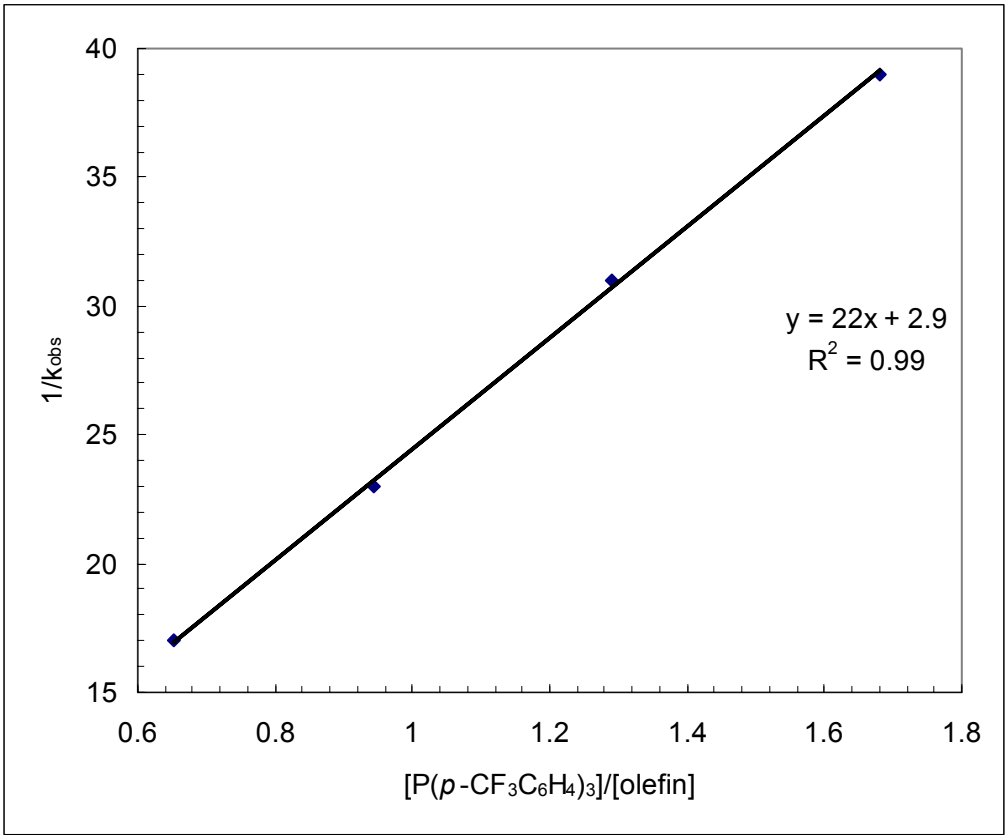


Figure S3. $1/k_{obs}$ vs. [P(*p*-$ClC_6H_4)_3$]/[olefin] for Catalyst **7**

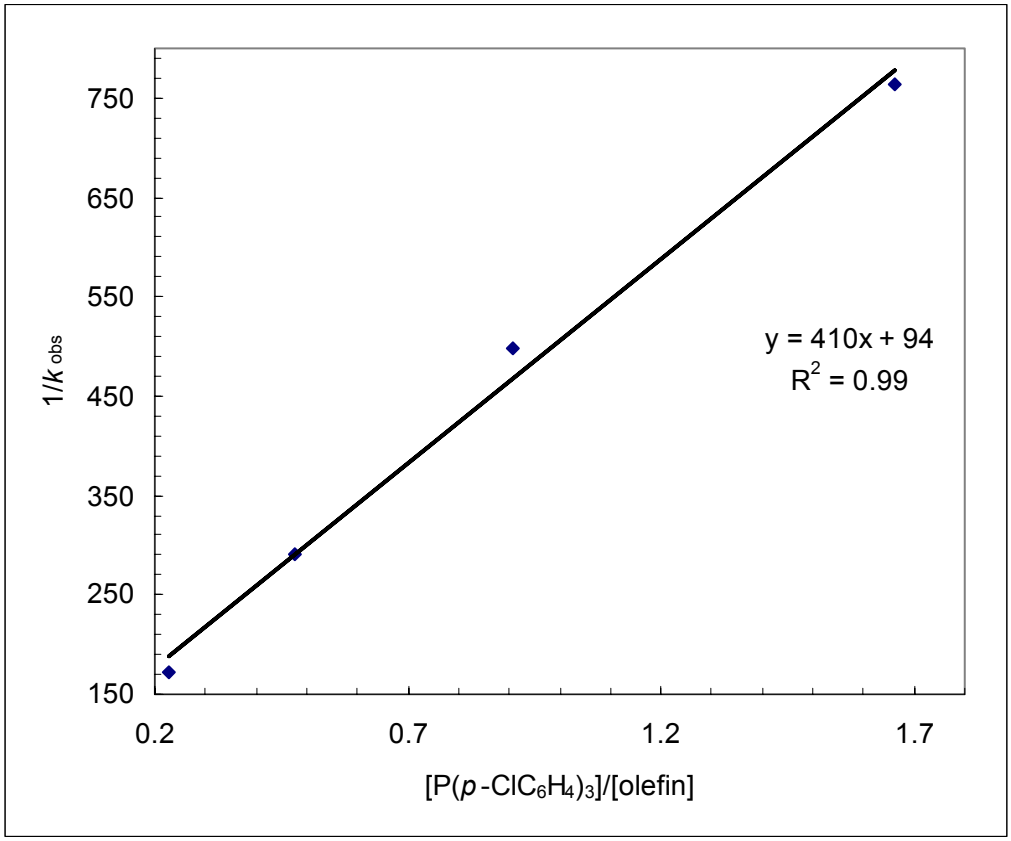


Figure S4. $1/k_{obs}$ vs. [P(*p*-FC_6H_4)$_3$]/[olefin] for Catalyst **8**

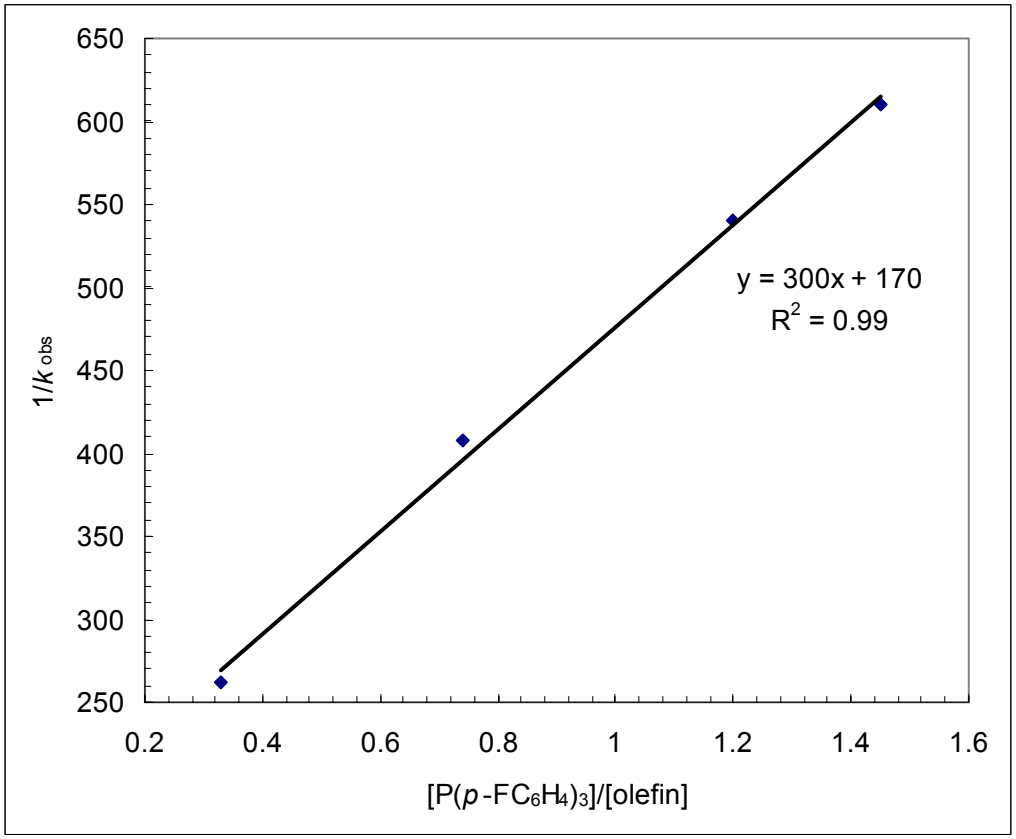


Figure S5. $1/k_{obs}$ vs. $[PPh_3]/[olefin]$ for Catalyst **9**

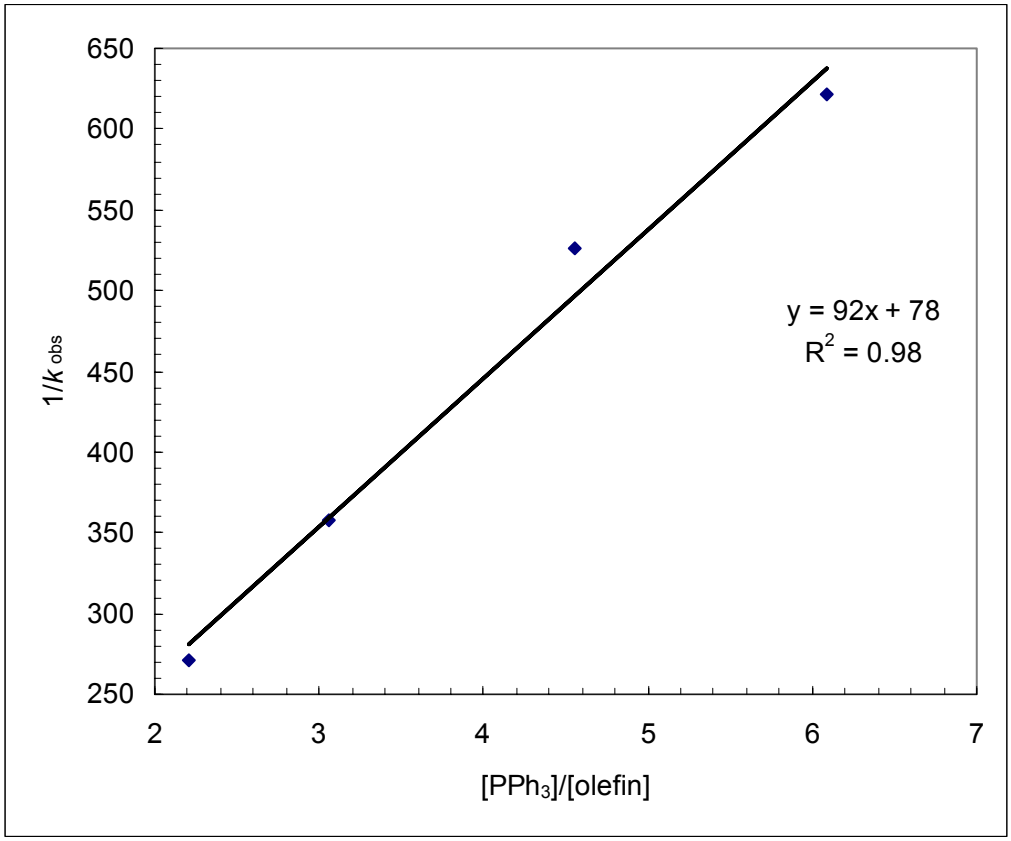


Figure S6. $1/k_{obs}$ vs. [P(p-$CH_3C_6H_4)_3$]/[olefin] for Catalyst **10**

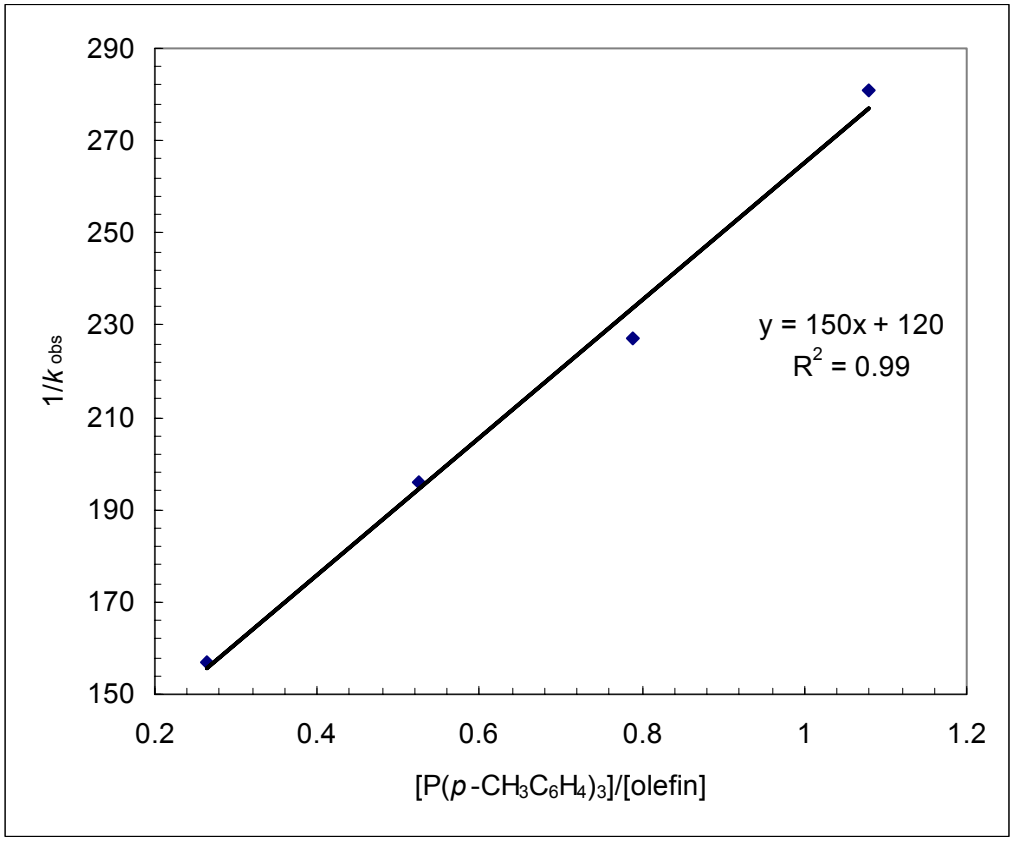


Figure S7. $1/k_{obs}$ vs. [P(*p*-$CH_3OC_6H_4)_3$]/[olefin] for Catalyst **11**

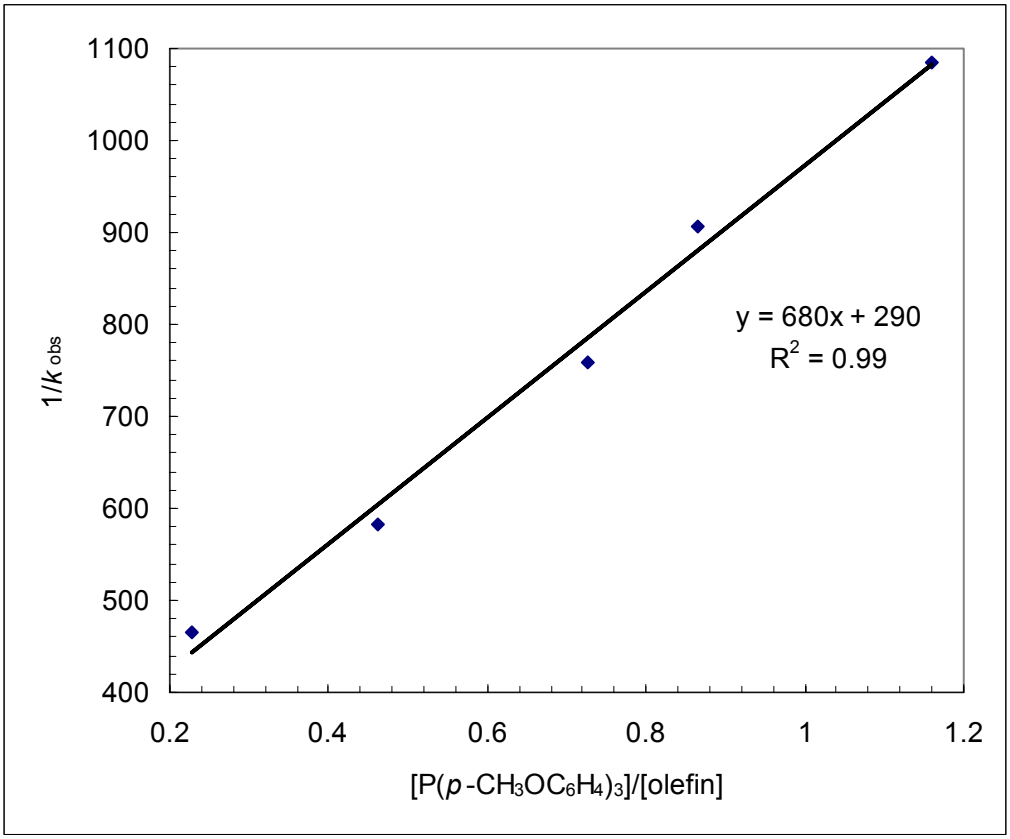


Figure S8. $1/k_1$ vs. ^{FT}X

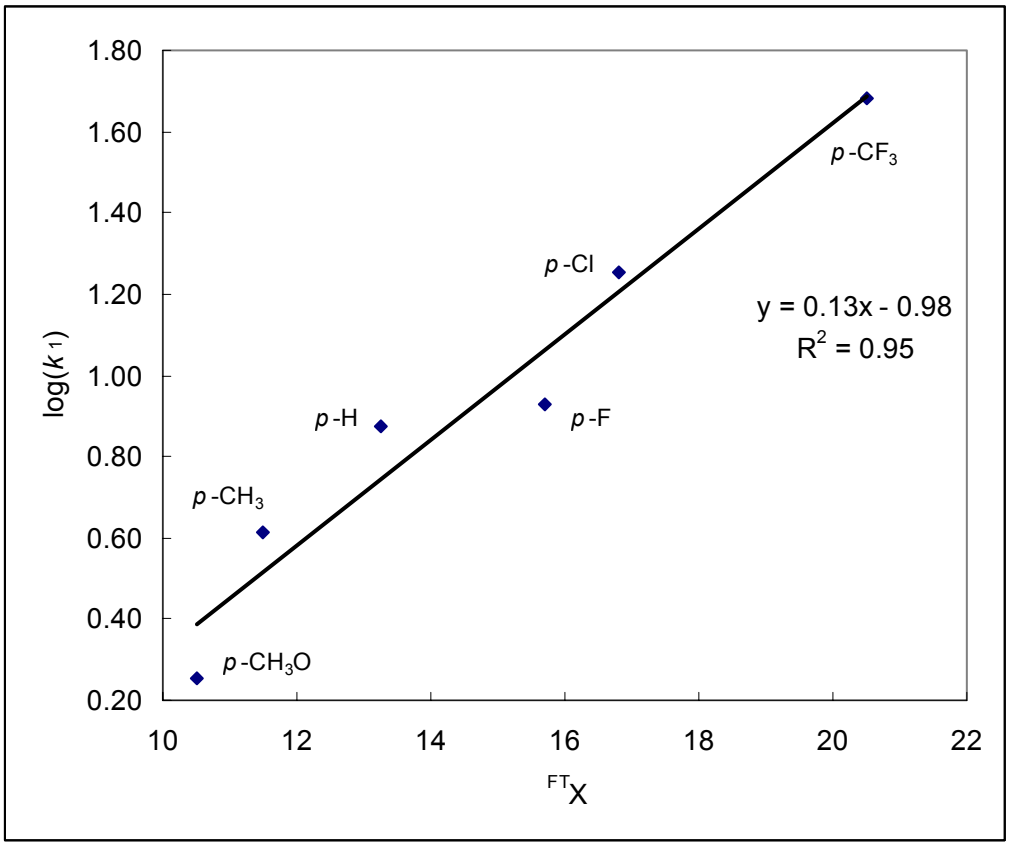


Figure S9. Eyring Plot for Initiation in Catalyst **4**

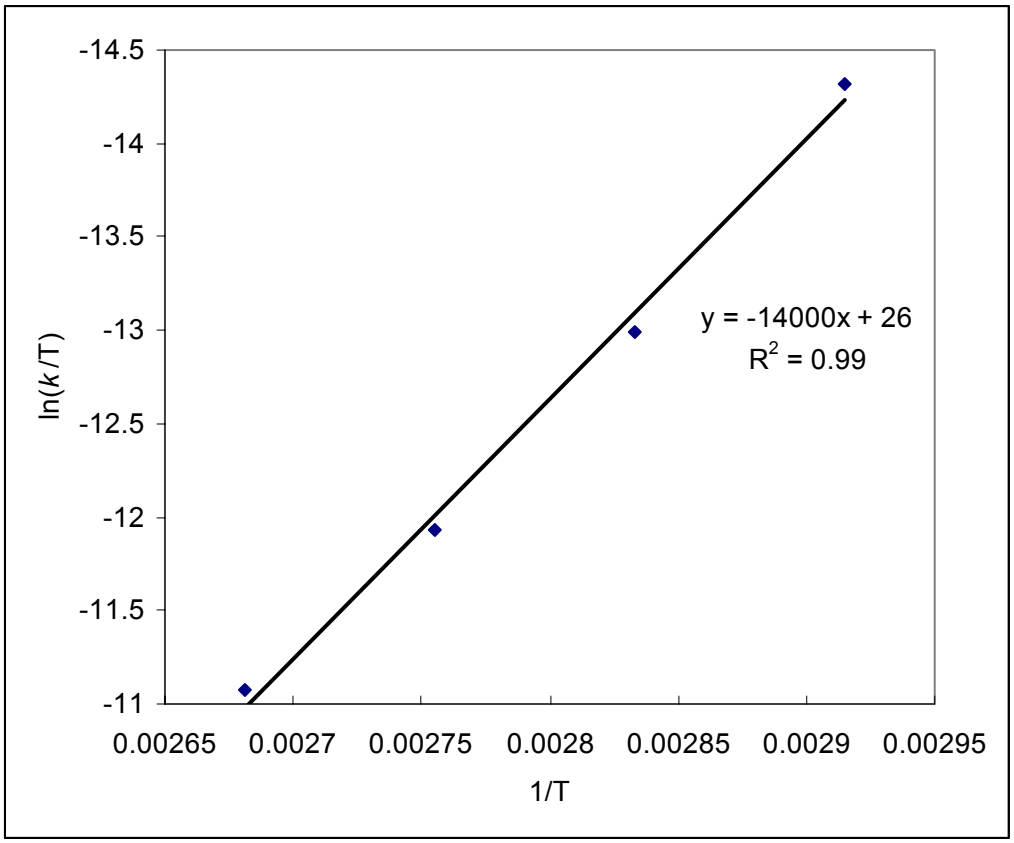


Figure S10. Eyring Plot for Initiation in Catalyst **14**

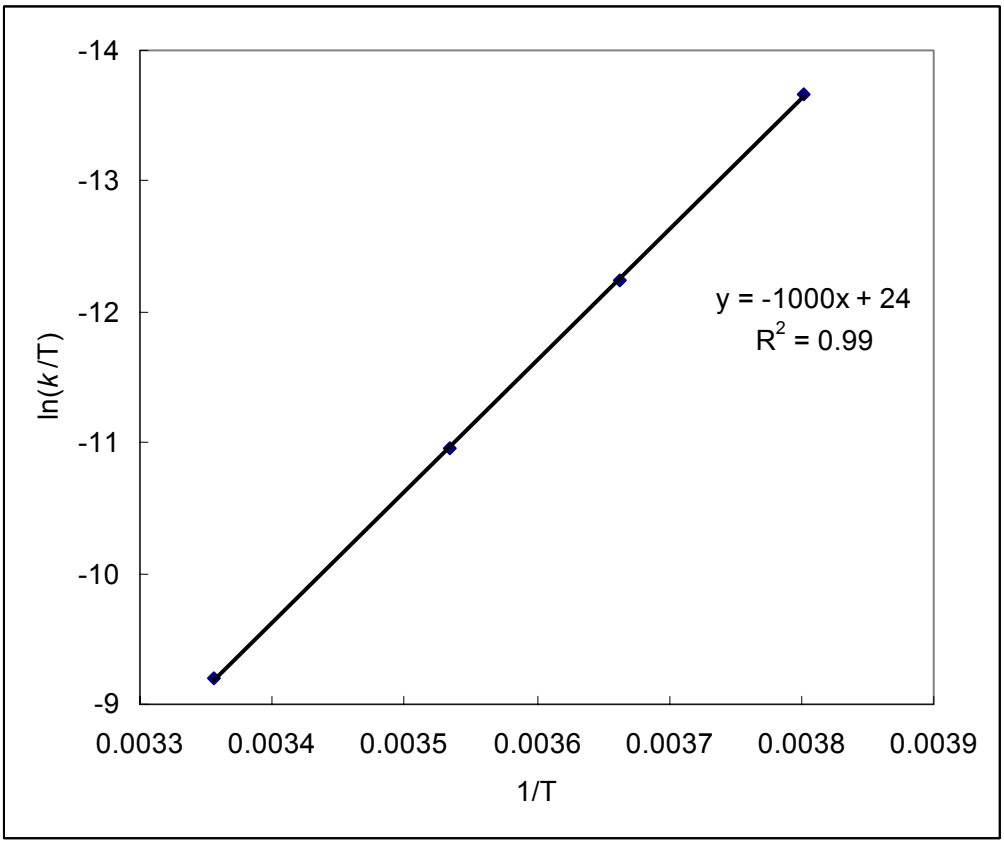


Figure S11. Dependence of Rate Constant on Olefin Concentration

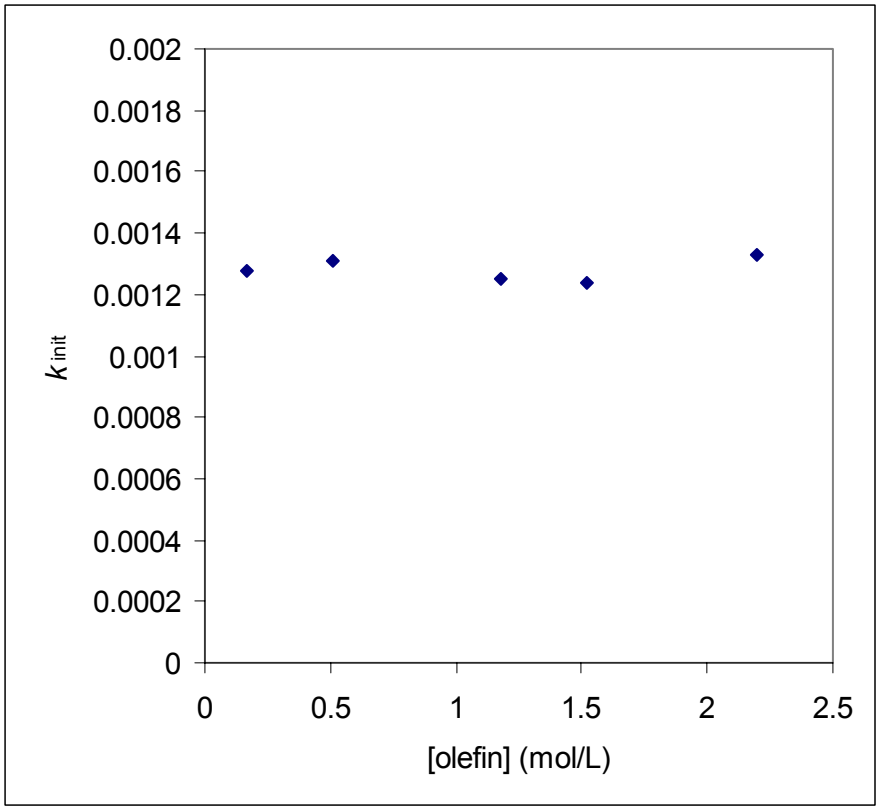


Figure S12. Crystal Structure of Complex **2**

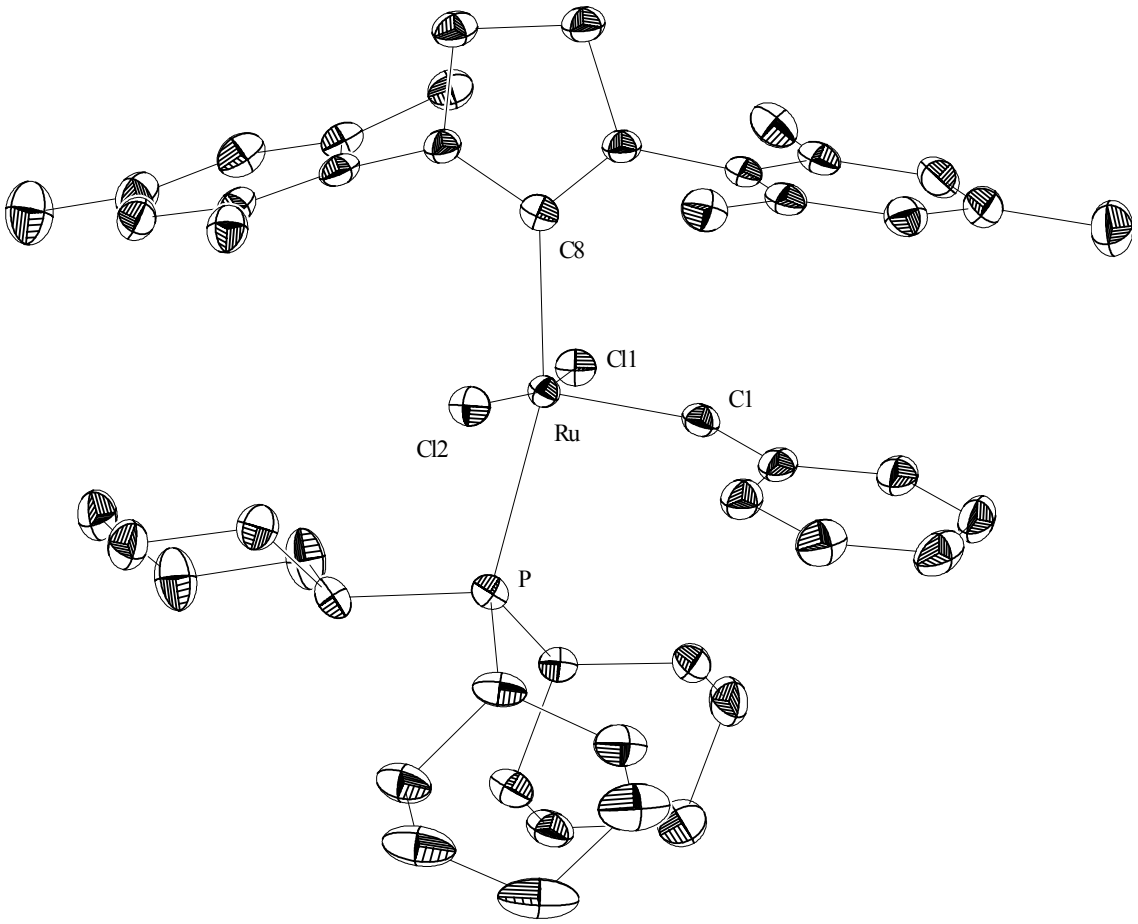


Table S5. Crystal Data and Structure Analysis Details for Complex 2.

Empirical formula	$C_{54.50}H_{77}Cl_2N_2PRu$ $[C_{46}H_{65}Cl_2N_2PRu \cdot C_6H_6 \cdot 0.5(C_5H_{12})]$
Formula weight	963.17 [836.97 ·78.11 ·0.5(72.15)]
Crystallization solvent	pentane / dichloromethane
Crystal shape	block
Crystal color	burgundy
Crystal size	0.21 x 0.26 x 0.30 mm

Data Collection

Preliminary photograph(s)	rotation	
Type of diffractometer	Bruker SMART 1000 ccd	
Wavelength	0.71073 Å MoKα	
Data collection temperature	98 K	
Theta range for 7485 reflections used in lattice determination	2.4 to 28.3°	
Unit cell dimensions	a = 12.2949(7) Å b = 14.9666(8) Å c = 27.1432(15) Å	α= 90° β= 97.601(1)° γ = 90°
Volume	4950.8(5) $Å^3$	
Z	4	
Crystal system	monoclinic	
Space group	P $2_1/n$ (# 14)	
Density (calculated)	1.292 g/cm^3	
F(000)	2044	
Theta range for data collection	1.5 to 28.5°	
Completeness to theta = 28.54°	94.5%	
Index ranges	$-16 \le h \le 16$, $-19 \le k \le 19$, $-34 \le l \le 34$	
Data collection scan type	ω scans at 6 fixed ϕ values	
Reflections collected	87057	
Independent reflections	11892 [R_{int}= 0.0465]	
Reflections > 2σ(I)	10104	
Average σ(I)/(net I)	0.0271	
Absorption coefficient	0.49 mm^{-1}	
Absorption correction	integration, empirical	
Max. and min. transmission	0.909 and 0.863 (and 0.934 from SADABS)	
Reflections monitored for decay	first 75 scans recollected at end of runs	
Decay of standards	within counting statistics	

Table S5 (cont.)

Structure Solution and Refinement

Primary solution method	direct methods
Secondary solution method	difference map
Hydrogen placement	calculated
Refinement method	full-matrix least-squares on F^2
Data / restraints / parameters	11892 / 0 / 751
Treatment of hydrogen atoms	mixed
Goodness-of-fit on F^2	2.66
Final R indices [I>2σ(I), 10104 reflections]	R1 = 0.0374, wR2 = 0.0764
R indices (all data)	R1 = 0.0479, wR2 = 0.0782
Type of weighting scheme used	sigma
Weighting scheme used	$w=1/\sigma^2(Fo^2)$
Max shift/error	0.050
Average shift/error	0.002
Largest diff. peak and hole	0.99 and -1.03 e·Å^{-3}

Programs Used

Cell refinement	Bruker SMART v5.606, Bruker SAINT v6.02
Data collection	Bruker SMART v5.054
Data reduction	Bruker SAINT v6.02
Absorption	Bruker SHELXTL v5.1, SADABS v2.03
Structure solution	SHELX-97 (Sheldrick, 1997)
Structure refinement	SHELX-97 (Sheldrick, 1997)
Graphics	Diamond, Bruker SHELXTL v5.1

References

Bruker (1999) SMART (v5.054), SMART (v5.606), SAINT (v6.02) and SHELXTL (v5.1). Bruker AXS Inc., Madison, Wisconsin, USA.

Diamond 2.1. (2000) Crystal Impact GbR, Bonn, Germany.

Spek, A.L. (1990). *Acta Cryst.,* A**46**, C-34.

Sheldrick, G. M. (1997). SHELXL-97. Program for Structures Refinement. Univ. of Gottingen, Federal Republic of Germany.

Special Refinement Details

A multifaceted burgundy block was selected from a batch of crystals, many with roughly rhombic cross-sections, and mounted on a glass fiber with Paratone-N oil. Six runs of data were collected with 20 second long, –0.25° wide ω–scans at six values of φ (0, 120, 240, 60, 180, and 300°) with the detector 5 cm (nominal) distant at a θ of -28°. The initial cell for data reduction was calculated from 999 centered reflections (4 eliminated in refinement) chosen from throughout the data frames. For data processing with SAINT v6.02, all defaults were used, except: a fixed box size of 1.8 x 1.8 x 0.75 was used, periodic orientation matrix updating was disabled, the instrument error was set to zero, no Laue class integration restraints were used, and for the post-integration global least squares refinement, no constraints were applied. No decay correction was needed. The larger faces of the crystal were indexed but a few minor ones could not be discerned clearly and were ignored. Absorption corrections were applied first from an integration based on the face-indexing (transmission: 0.909 to 0.863) and subsequently with a SADABS correction (relative values: 1.000 to 0.934) using v2.03 with g=0.0635 and all defaults.

No reflections were specifically omitted from the final processed dataset; 1811 reflections were rejected, with 11 space group-absence violations, 0 inconsistent equivalents, and no reflections suppressed. Refinement of F^2 was against all reflections. The weighted R-factor (*w*R) and goodness of fit (S) are based on F^2, conventional R-factors (R) are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement.

The asymmetric unit consists of one molecule of the compound, a molecule of benzene, and ½ molecule of n-pentane. The five-coordinate Ru has distorted square-pyramidal geometry (Cl(1)-Ru-Cl(2) = 167.707(18)° and C(1)-Ru-P = 163.73(6)°) with the benzylidene carbene (Ru-C(22) = 1.835(2)Å) at the apex (C(22)-Ru-C(1) = 100.24(8)°, C(22)-Ru-Cl(1) = 103.15(7)°, C(22)-Ru-Cl(2) = 89.14(7)°, and C(22)-Ru-P = 95.89(6)°). The $RuCl_2$ plane forms an angle of 13(2)° with the Ru-C22-H22 plane. The two phenyl groups of the N-heterocyclic carbene form angles of 87.64(6)° and 81.52(6)° with the N_2C_3 plane and an angle of 21.68(10)° with respect to one another.
The benzene pivots around two atoms; the other four have large in-plane displacements. Splitting these atoms produced no improvement. The pentane is disordered over a center of symmetry. The two orientations essentially share the center carbon and terminal methyl groups; the other two atoms were split over two sites each. No restraints or constraints were used. All heavy atoms were refined anisotropically. The solvents form layers perpendicular to the c-axis at z ~ 0, ½, and 1, but do not appear to interact. The coordinates of the hydrogen atoms on the molecule were refined and those on the solvent molecules fixed at calculated values; all hydrogen U_{iso}'s were set at 120% of the U_{eq}'s of the attached atoms. The coordinates of H20B were slow to converge. In the final difference map, the largest positive peak of 0.99 e·Å^{-3} was 0.34 Å from C51 and the largest negative peak of –1.03 e·Å^{-3} was 0.27 Å from C51; this is one of the smeared out benzene atoms. Analysis of intermolecular contacts with Platon shows a few borderline interactions, primarily involving hydrogen atoms of the solvents.

Table S6. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for Complex 2. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
Ru	-207(1)	380(1)	2109(1)	14(1)
Cl(1)	1266(1)	1406(1)	2334(1)	21(1)
Cl(2)	-1656(1)	-701(1)	2071(1)	19(1)
P	1070(1)	-857(1)	2125(1)	18(1)
N(1)	-1321(1)	1613(1)	2783(1)	19(1)
N(2)	-1590(1)	2122(1)	2028(1)	19(1)
C(1)	-1166(2)	1434(1)	2311(1)	17(1)
C(2)	-1829(2)	2493(1)	2843(1)	23(1)
C(3)	-2133(2)	2799(2)	2310(1)	23(1)
C(4)	-1200(2)	1012(1)	3201(1)	20(1)
C(5)	-295(2)	1075(1)	3566(1)	21(1)
C(6)	-268(2)	521(1)	3983(1)	25(1)
C(7)	-1104(2)	-65(2)	4044(1)	28(1)
C(8)	-2013(2)	-85(2)	3679(1)	26(1)
C(9)	-2092(2)	449(1)	3260(1)	21(1)
C(10)	624(2)	1724(2)	3536(1)	26(1)
C(11)	-1036(3)	-673(2)	4490(1)	40(1)
C(12)	-3110(2)	453(2)	2890(1)	24(1)
C(13)	-1756(2)	2190(1)	1497(1)	19(1)
C(14)	-2655(2)	1749(1)	1232(1)	22(1)
C(15)	-2840(2)	1859(2)	719(1)	27(1)
C(16)	-2178(2)	2397(1)	469(1)	28(1)
C(17)	-1311(2)	2843(2)	745(1)	25(1)
C(18)	-1086(2)	2753(1)	1259(1)	21(1)
C(19)	-3397(2)	1166(2)	1493(1)	27(1)
C(20)	-2395(3)	2493(2)	-88(1)	41(1)
C(21)	-143(2)	3242(2)	1546(1)	26(1)
C(22)	-460(2)	479(1)	1429(1)	18(1)
C(23)	99(2)	873(1)	1035(1)	21(1)
C(24)	-401(2)	754(1)	543(1)	25(1)
C(25)	76(2)	1092(2)	145(1)	31(1)
C(26)	1055(2)	1546(2)	228(1)	33(1)
C(27)	1561(2)	1673(2)	710(1)	31(1)
C(28)	1095(2)	1344(1)	1109(1)	24(1)
C(29)	578(2)	-1902(1)	1806(1)	19(1)
C(30)	54(2)	-1839(1)	1265(1)	24(1)
C(31)	-527(2)	-2720(2)	1112(1)	31(1)
C(32)	266(2)	-3509(2)	1180(1)	32(1)
C(33)	837(2)	-3559(1)	1711(1)	26(1)
C(34)	1405(2)	-2680(1)	1874(1)	24(1)
C(35)	2422(2)	-543(1)	1938(1)	25(1)
C(36)	2435(2)	-643(2)	1377(1)	30(1)
C(37)	3468(2)	-230(2)	1217(1)	44(1)
C(38)	4491(2)	-644(2)	1505(1)	44(1)

C(39)	4486(2)	-570(2)	2055(1)	41(1)
C(40)	3452(2)	-978(2)	2223(1)	31(1)
C(41)	1409(2)	-1260(1)	2775(1)	21(1)
C(42)	1695(2)	-482(2)	3132(1)	26(1)
C(43)	2118(2)	-816(2)	3652(1)	31(1)
C(44)	1309(2)	-1444(2)	3849(1)	33(1)
C(45)	963(2)	-2196(2)	3487(1)	36(1)
C(46)	529(2)	-1841(2)	2969(1)	32(1)
C(47)	6513(2)	7706(2)	666(1)	49(1)
C(48)	6834(2)	8516(2)	824(1)	37(1)
C(49)	6631(3)	9231(2)	522(2)	67(1)
C(50)	6076(4)	9100(4)	36(2)	121(3)
C(51)	5788(3)	8225(5)	-99(1)	119(3)
C(52)	6007(3)	7570(3)	212(2)	90(2)
C(53)	8157(5)	5848(3)	16(2)	105(2)
C(54)[a]	8945(8)	5034(5)	77(3)	71(2)
C(55)	10000	5000	0	97(3)
C(56)[a]	10824(6)	4165(4)	96(2)	51(2)

[a] Population: ½

Table S7. Selected bond lengths [Å] and angles [°] for Complex 2.

Ru-C(22)	1.835(2)	C(22)-Ru-C(1)	100.24(8)
Ru-C(1)	2.0847(19)	C(22)-Ru-Cl(1)	103.15(7)
Ru-Cl(1)	2.3912(5)	C(1)-Ru-Cl(1)	83.26(5)
Ru-Cl(2)	2.3988(5)	C(22)-Ru-Cl(2)	89.14(7)
Ru-P	2.4245(5)	C(1)-Ru-Cl(2)	94.55(5)
C(22)-C(23)	1.470(3)	Cl(1)-Ru-Cl(2)	167.707(18)
		C(22)-Ru-P	95.89(6)
		C(1)-Ru-P	163.73(6)
		Cl(1)-Ru-P	91.063(18)
		Cl(2)-Ru-P	87.753(18)
		C(23)-C(22)-Ru	136.98(16)
		Ru-C(22)-H(22)	112.6(13)

Table S8. Bond lengths [Å] and angles [°] for Complex 2.

Ru-C(22)	1.835(2)	C(19)-H(19A)	0.97(2)
Ru-C(1)	2.0847(19)	C(19)-H(19B)	0.97(2)
Ru-Cl(1)	2.3912(5)	C(19)-H(19C)	0.89(2)
Ru-Cl(2)	2.3988(5)	C(20)-H(20A)	0.85(3)
Ru-P	2.4245(5)	C(20)-H(20B)	0.90(3)
P-C(29)	1.850(2)	C(20)-H(20C)	0.83(3)
P-C(41)	1.859(2)	C(21)-H(21A)	0.91(2)
P-C(35)	1.861(2)	C(21)-H(21B)	0.93(2)
N(1)-C(1)	1.347(2)	C(21)-H(21C)	0.95(2)
N(1)-C(4)	1.440(2)	C(22)-C(23)	1.470(3)
N(1)-C(2)	1.476(2)	C(22)-H(22)	0.93(2)
N(2)-C(1)	1.348(2)	C(23)-C(28)	1.404(3)
N(2)-C(13)	1.432(2)	C(23)-C(24)	1.406(3)
N(2)-C(3)	1.482(3)	C(24)-C(25)	1.390(3)
C(2)-C(3)	1.515(3)	C(24)-H(24)	0.94(2)
C(2)-H(2A)	0.96(2)	C(25)-C(26)	1.374(3)
C(2)-H(2B)	0.95(2)	C(25)-H(25)	0.92(2)
C(3)-H(3A)	0.92(2)	C(26)-C(27)	1.387(3)
C(3)-H(3B)	0.98(2)	C(26)-H(26)	0.93(2)
C(4)-C(5)	1.393(3)	C(27)-C(28)	1.382(3)
C(4)-C(9)	1.409(3)	C(27)-H(27)	0.97(2)
C(5)-C(6)	1.399(3)	C(28)-H(28)	0.95(2)
C(5)-C(10)	1.501(3)	C(29)-C(30)	1.527(3)
C(6)-C(7)	1.378(3)	C(29)-C(34)	1.541(3)
C(6)-H(6)	0.95(2)	C(29)-H(29)	0.86(2)
C(7)-C(8)	1.393(3)	C(30)-C(31)	1.531(3)
C(7)-C(11)	1.507(3)	C(30)-H(30A)	0.96(2)
C(8)-C(9)	1.382(3)	C(30)-H(30B)	0.94(2)
C(8)-H(8)	0.90(2)	C(31)-C(32)	1.526(3)
C(9)-C(12)	1.497(3)	C(31)-H(31A)	1.01(2)
C(10)-H(10A)	0.96(2)	C(31)-H(31B)	0.92(2)
C(10)-H(10B)	0.91(2)	C(32)-C(33)	1.518(3)
C(10)-H(10C)	0.86(2)	C(32)-H(32A)	0.94(2)
C(11)-H(11A)	0.92(3)	C(32)-H(32B)	1.00(2)
C(11)-H(11B)	0.93(3)	C(33)-C(34)	1.528(3)
C(11)-H(11C)	0.88(3)	C(33)-H(33A)	0.93(2)
C(12)-H(12A)	0.93(2)	C(33)-H(33B)	0.99(2)
C(12)-H(12B)	0.93(2)	C(34)-H(34A)	1.02(2)
C(12)-H(12C)	0.96(2)	C(34)-H(34B)	1.00(2)
C(13)-C(18)	1.394(3)	C(35)-C(36)	1.531(3)
C(13)-C(14)	1.402(3)	C(35)-C(40)	1.540(3)
C(14)-C(15)	1.391(3)	C(35)-H(35)	0.97(2)
C(14)-C(19)	1.503(3)	C(36)-C(37)	1.528(3)
C(15)-C(16)	1.385(3)	C(36)-H(36A)	0.97(2)
C(15)-H(15)	0.93(2)	C(36)-H(36B)	0.94(2)
C(16)-C(17)	1.389(3)	C(37)-C(38)	1.522(4)
C(16)-C(20)	1.506(3)	C(37)-H(37A)	0.93(3)
C(17)-C(18)	1.392(3)	C(37)-H(37B)	1.00(3)
C(17)-H(17)	0.91(2)	C(38)-C(39)	1.499(4)
C(18)-C(21)	1.500(3)	C(38)-H(38A)	0.98(3)

C(38)-H(38B)	0.92(3)	C(55)-H(55A)	0.96
C(39)-C(40)	1.532(3)	C(55)-H(55B)	0.96
C(39)-H(39A)	0.99(3)	C(55)-H(55C)^{i}	0.96
C(39)-H(39B)	0.97(3)	C(55)-H(55D)^{i}	0.96
C(40)-H(40A)	1.00(2)	C(56)-C(53)^{i}	1.328(7)
C(40)-H(40B)	0.95(2)	C(56)-H(56A)	0.96
C(41)-C(42)	1.526(3)	C(56)-H(56B)	0.96
C(41)-C(46)	1.534(3)	C(56)-H(56C)^{i}	0.96
C(41)-H(41)	0.93(2)	C(56)-H(56D)^{i}	0.96
C(42)-C(43)	1.522(3)		
C(42)-H(42A)	0.93(2)	C(22)-Ru-C(1)	100.24(8)
C(42)-H(42B)	0.95(2)	C(22)-Ru-Cl(1)	103.15(7)
C(43)-C(44)	1.517(3)	C(1)-Ru-Cl(1)	83.26(5)
C(43)-H(43A)	0.92(2)	C(22)-Ru-Cl(2)	89.14(7)
C(43)-H(43B)	0.98(2)	C(1)-Ru-Cl(2)	94.55(5)
C(44)-C(45)	1.516(3)	Cl(1)-Ru-Cl(2)	167.707(18)
C(44)-H(44A)	0.98(2)	C(22)-Ru-P	95.89(6)
C(44)-H(44B)	0.98(2)	C(1)-Ru-P	163.73(6)
C(45)-C(46)	1.532(3)	Cl(1)-Ru-P	91.063(18)
C(45)-H(45A)	1.00(3)	Cl(2)-Ru-P	87.753(18)
C(45)-H(45B)	0.98(3)	C(29)-P-C(41)	100.84(9)
C(46)-H(46A)	1.00(2)	C(29)-P-C(35)	109.54(10)
C(46)-H(46B)	1.01(2)	C(41)-P-C(35)	104.17(10)
C(47)-C(52)	1.321(5)	C(29)-P-Ru	117.78(7)
C(47)-C(48)	1.328(4)	C(41)-P-Ru	109.17(7)
C(47)-H(47)	0.9500	C(35)-P-Ru	113.69(7)
C(48)-C(49)	1.350(4)	C(1)-N(1)-C(4)	127.74(16)
C(48)-H(48)	0.9500	C(1)-N(1)-C(2)	113.49(16)
C(49)-C(50)	1.418(6)	C(4)-N(1)-C(2)	118.10(15)
C(49)-H(49)	0.9500	C(1)-N(2)-C(13)	128.39(16)
C(50)-C(51)	1.392(7)	C(1)-N(2)-C(3)	113.20(16)
C(50)-H(50)	0.9500	C(13)-N(2)-C(3)	117.26(16)
C(51)-C(52)	1.299(7)	N(1)-C(1)-N(2)	107.27(16)
C(51)-H(51)	0.9500	N(1)-C(1)-Ru	123.90(14)
C(52)-H(52)	0.9500	N(2)-C(1)-Ru	128.08(14)
C(53)-C(54)	1.552(9)	N(1)-C(2)-C(3)	102.64(16)
C(53)-H(53A)	0.96	N(1)-C(2)-H(2A)	109.3(13)
C(53)-H(53B)	0.96	C(3)-C(2)-H(2A)	112.9(13)
C(53)-H(53C)	0.96	N(1)-C(2)-H(2B)	111.1(13)
C(53)-H(53D)	0.96	C(3)-C(2)-H(2B)	110.2(13)
C(53)-H(53E)	0.96	H(2A)-C(2)-H(2B)	110.4(19)
C(53)-H(53F)	0.96	N(2)-C(3)-C(2)	102.47(16)
C(53)-H(53G)	0.96	N(2)-C(3)-H(3A)	108.3(14)
C(53)-H(53H)	0.96	C(2)-C(3)-H(3A)	113.1(14)
C(53)-H(53I)	0.96	N(2)-C(3)-H(3B)	110.7(13)
C(53)-H(53J)	0.96	C(2)-C(3)-H(3B)	114.0(13)
C(53)-H(53K)	0.96	H(3A)-C(3)-H(3B)	108.1(19)
C(53)-H(53L)	0.96	C(5)-C(4)-C(9)	121.31(18)
C(54)-C(55)	1.342(9)	C(5)-C(4)-N(1)	120.59(18)
C(54)-H(54A)	0.96	C(9)-C(4)-N(1)	117.55(18)
C(54)-H(54B)	0.96	C(4)-C(5)-C(6)	117.84(19)
C(55)-C(56)	1.608(8)	C(4)-C(5)-C(10)	122.77(19)

C(6)-C(5)-C(10)	119.37(19)	C(14)-C(19)-H(19C)	111.5(15)
C(7)-C(6)-C(5)	122.4(2)	H(19A)-C(19)-H(19C)	111(2)
C(7)-C(6)-H(6)	119.0(14)	H(19B)-C(19)-H(19C)	105(2)
C(5)-C(6)-H(6)	118.6(14)	C(16)-C(20)-H(20A)	114.8(19)
C(6)-C(7)-C(8)	118.0(2)	C(16)-C(20)-H(20B)	112.3(18)
C(6)-C(7)-C(11)	121.1(2)	H(20A)-C(20)-H(20B)	108(3)
C(8)-C(7)-C(11)	120.8(2)	C(16)-C(20)-H(20C)	111(2)
C(9)-C(8)-C(7)	122.3(2)	H(20A)-C(20)-H(20C)	113(3)
C(9)-C(8)-H(8)	116.4(15)	H(20B)-C(20)-H(20C)	96(2)
C(7)-C(8)-H(8)	121.2(15)	C(18)-C(21)-H(21A)	111.7(14)
C(8)-C(9)-C(4)	117.95(19)	C(18)-C(21)-H(21B)	113.1(14)
C(8)-C(9)-C(12)	121.00(19)	H(21A)-C(21)-H(21B)	107(2)
C(4)-C(9)-C(12)	121.01(19)	C(18)-C(21)-H(21C)	113.9(14)
C(5)-C(10)-H(10A)	113.6(14)	H(21A)-C(21)-H(21C)	106(2)
C(5)-C(10)-H(10B)	113.4(14)	H(21B)-C(21)-H(21C)	104.3(19)
H(10A)-C(10)-H(10B)	103.2(19)	C(23)-C(22)-Ru	136.98(16)
C(5)-C(10)-H(10C)	110.2(16)	C(23)-C(22)-H(22)	110.4(13)
H(10A)-C(10)-H(10C)	110(2)	Ru-C(22)-H(22)	112.6(13)
H(10B)-C(10)-H(10C)	106(2)	C(28)-C(23)-C(24)	117.57(19)
C(7)-C(11)-H(11A)	113.3(17)	C(28)-C(23)-C(22)	125.40(19)
C(7)-C(11)-H(11B)	110.2(16)	C(24)-C(23)-C(22)	117.02(19)
H(11A)-C(11)-H(11B)	105(2)	C(25)-C(24)-C(23)	121.1(2)
C(7)-C(11)-H(11C)	112.0(18)	C(25)-C(24)-H(24)	120.3(14)
H(11A)-C(11)-H(11C)	106(2)	C(23)-C(24)-H(24)	118.6(14)
H(11B)-C(11)-H(11C)	109(2)	C(26)-C(25)-C(24)	120.2(2)
C(9)-C(12)-H(12A)	110.5(14)	C(26)-C(25)-H(25)	119.8(15)
C(9)-C(12)-H(12B)	111.3(14)	C(24)-C(25)-H(25)	120.0(15)
H(12A)-C(12)-H(12B)	109.0(19)	C(25)-C(26)-C(27)	119.8(2)
C(9)-C(12)-H(12C)	113.8(13)	C(25)-C(26)-H(26)	120.1(15)
H(12A)-C(12)-H(12C)	106.4(19)	C(27)-C(26)-H(26)	120.1(15)
H(12B)-C(12)-H(12C)	105.5(19)	C(28)-C(27)-C(26)	120.6(2)
C(18)-C(13)-C(14)	121.44(19)	C(28)-C(27)-H(27)	120.2(14)
C(18)-C(13)-N(2)	119.66(18)	C(26)-C(27)-H(27)	119.2(14)
C(14)-C(13)-N(2)	118.64(18)	C(27)-C(28)-C(23)	120.7(2)
C(15)-C(14)-C(13)	118.0(2)	C(27)-C(28)-H(28)	119.8(13)
C(15)-C(14)-C(19)	120.7(2)	C(23)-C(28)-H(28)	119.4(13)
C(13)-C(14)-C(19)	121.29(19)	C(30)-C(29)-C(34)	110.41(17)
C(16)-C(15)-C(14)	122.1(2)	C(30)-C(29)-P	117.90(14)
C(16)-C(15)-H(15)	121.0(14)	C(34)-C(29)-P	114.42(14)
C(14)-C(15)-H(15)	116.9(14)	C(30)-C(29)-H(29)	106.5(14)
C(15)-C(16)-C(17)	118.3(2)	C(34)-C(29)-H(29)	106.6(14)
C(15)-C(16)-C(20)	120.6(2)	P-C(29)-H(29)	99.5(14)
C(17)-C(16)-C(20)	121.1(2)	C(29)-C(30)-C(31)	109.25(18)
C(16)-C(17)-C(18)	122.0(2)	C(29)-C(30)-H(30A)	112.3(14)
C(16)-C(17)-H(17)	121.9(15)	C(31)-C(30)-H(30A)	108.0(13)
C(18)-C(17)-H(17)	116.1(15)	C(29)-C(30)-H(30B)	109.7(14)
C(17)-C(18)-C(13)	118.1(2)	C(31)-C(30)-H(30B)	110.6(13)
C(17)-C(18)-C(21)	120.7(2)	H(30A)-C(30)-H(30B)	107.0(18)
C(13)-C(18)-C(21)	121.13(19)	C(32)-C(31)-C(30)	111.5(2)
C(14)-C(19)-H(19A)	110.0(14)	C(32)-C(31)-H(31A)	108.4(13)
C(14)-C(19)-H(19B)	113.1(14)	C(30)-C(31)-H(31A)	109.4(14)
H(19A)-C(19)-H(19B)	106.3(19)	C(32)-C(31)-H(31B)	110.3(15)

C(30)-C(31)-H(31B)	109.2(15)
H(31A)-C(31)-H(31B)	108(2)
C(33)-C(32)-C(31)	111.17(19)
C(33)-C(32)-H(32A)	109.7(15)
C(31)-C(32)-H(32A)	110.0(15)
C(33)-C(32)-H(32B)	107.7(14)
C(31)-C(32)-H(32B)	110.0(14)
H(32A)-C(32)-H(32B)	108(2)
C(32)-C(33)-C(34)	111.61(19)
C(32)-C(33)-H(33A)	111.5(14)
C(34)-C(33)-H(33A)	107.8(14)
C(32)-C(33)-H(33B)	111.6(13)
C(34)-C(33)-H(33B)	109.6(13)
H(33A)-C(33)-H(33B)	104.4(19)
C(33)-C(34)-C(29)	110.35(17)
C(33)-C(34)-H(34A)	108.6(12)
C(29)-C(34)-H(34A)	109.6(12)
C(33)-C(34)-H(34B)	111.1(12)
C(29)-C(34)-H(34B)	112.7(13)
H(34A)-C(34)-H(34B)	104.1(17)
C(36)-C(35)-C(40)	109.98(19)
C(36)-C(35)-P	111.94(15)
C(40)-C(35)-P	117.49(16)
C(36)-C(35)-H(35)	107.8(13)
C(40)-C(35)-H(35)	107.4(13)
P-C(35)-H(35)	101.4(13)
C(37)-C(36)-C(35)	111.2(2)
C(37)-C(36)-H(36A)	107.4(14)
C(35)-C(36)-H(36A)	109.1(14)
C(37)-C(36)-H(36B)	109.7(14)
C(35)-C(36)-H(36B)	112.8(15)
H(36A)-C(36)-H(36B)	106(2)
C(38)-C(37)-C(36)	110.5(2)
C(38)-C(37)-H(37A)	109.7(17)
C(36)-C(37)-H(37A)	105.9(17)
C(38)-C(37)-H(37B)	113.1(15)
C(36)-C(37)-H(37B)	108.2(16)
H(37A)-C(37)-H(37B)	109(2)
C(39)-C(38)-C(37)	111.7(2)
C(39)-C(38)-H(38A)	108.1(16)
C(37)-C(38)-H(38A)	108.2(15)
C(39)-C(38)-H(38B)	110.1(17)
C(37)-C(38)-H(38B)	112.0(17)
H(38A)-C(38)-H(38B)	107(2)
C(38)-C(39)-C(40)	112.3(2)
C(38)-C(39)-H(39A)	113.7(15)
C(40)-C(39)-H(39A)	104.9(15)
C(38)-C(39)-H(39B)	110.1(16)
C(40)-C(39)-H(39B)	110.3(16)
H(39A)-C(39)-H(39B)	105(2)
C(39)-C(40)-C(35)	110.0(2)
C(39)-C(40)-H(40A)	109.8(14)
C(35)-C(40)-H(40A)	108.9(14)
C(39)-C(40)-H(40B)	110.1(14)
C(35)-C(40)-H(40B)	108.9(14)
H(40A)-C(40)-H(40B)	109(2)
C(42)-C(41)-C(46)	109.20(19)
C(42)-C(41)-P	111.06(14)
C(46)-C(41)-P	115.44(15)
C(42)-C(41)-H(41)	106.9(13)
C(46)-C(41)-H(41)	107.5(13)
P-C(41)-H(41)	106.3(13)
C(43)-C(42)-C(41)	111.12(19)
C(43)-C(42)-H(42A)	108.7(14)
C(41)-C(42)-H(42A)	107.4(14)
C(43)-C(42)-H(42B)	112.5(14)
C(41)-C(42)-H(42B)	111.0(14)
H(42A)-C(42)-H(42B)	105.8(19)
C(44)-C(43)-C(42)	111.7(2)
C(44)-C(43)-H(43A)	107.1(15)
C(42)-C(43)-H(43A)	109.8(15)
C(44)-C(43)-H(43B)	111.5(14)
C(42)-C(43)-H(43B)	110.7(14)
H(43A)-C(43)-H(43B)	106(2)
C(45)-C(44)-C(43)	111.9(2)
C(45)-C(44)-H(44A)	107.7(14)
C(43)-C(44)-H(44A)	108.5(14)
C(45)-C(44)-H(44B)	111.9(14)
C(43)-C(44)-H(44B)	108.3(14)
H(44A)-C(44)-H(44B)	108.4(19)
C(44)-C(45)-C(46)	111.8(2)
C(44)-C(45)-H(45A)	110.5(14)
C(46)-C(45)-H(45A)	111.0(14)
C(44)-C(45)-H(45B)	110.9(15)
C(46)-C(45)-H(45B)	109.4(15)
H(45A)-C(45)-H(45B)	103(2)
C(45)-C(46)-C(41)	109.62(19)
C(45)-C(46)-H(46A)	108.6(14)
C(41)-C(46)-H(46A)	108.4(14)
C(45)-C(46)-H(46B)	107.1(14)
C(41)-C(46)-H(46B)	112.2(14)
H(46A)-C(46)-H(46B)	111.0(19)
C(52)-C(47)-C(48)	121.7(3)
C(52)-C(47)-H(47)	119.2
C(48)-C(47)-H(47)	119.2
C(47)-C(48)-C(49)	120.3(3)
C(47)-C(48)-H(48)	119.9
C(49)-C(48)-H(48)	119.9
C(48)-C(49)-C(50)	118.8(3)
C(48)-C(49)-H(49)	120.6
C(50)-C(49)-H(49)	120.6
C(51)-C(50)-C(49)	116.7(3)
C(51)-C(50)-H(50)	121.6

C(49)-C(50)-H(50)	121.6
C(52)-C(51)-C(50)	121.0(4)
C(52)-C(51)-H(51)	119.5
C(50)-C(51)-H(51)	119.5
C(51)-C(52)-C(47)	121.4(4)
C(51)-C(52)-H(52)	119.3
C(47)-C(52)-H(52)	119.3
C(54)-C(53)-H(53A)	107.6
C(54)-C(53)-H(53B)	110.4
C(54)-C(53)-H(53C)	110.4
H(53A)-C(53)-H(53B)	109.5
H(53A)-C(53)-H(53C)	109.5
H(53B)-C(53)-H(53C)	109.5
H(53D)-C(53)-H(53E)	109.5
H(53D)-C(53)-H(53F)	109.5
H(53E)-C(53)-H(53F)	109.5
H(53G)^{i}-C(53)-H(53H)^{i}	109.5
H(53G)^{i}-C(53)-H(53I)^{i}	109.5
H(53H)^{i}-C(53)-H(53I)^{i}	109.5
H(53I)^{i}-C(53)-H(53J)^{i}	109.5
H(53I)^{i}-C(53)-H(53K)^{i}	109.5
H(53J)^{i}-C(53)-H(53K)^{i}	109.5
C(55)-C(54)-C(53)	128.1(6)
C(55)-C(54)-H(54A)	105.2
C(53)-C(54)-H(54A)	105.9
C(55)-C(54)-H(54B)	104.3
C(53)-C(54)-H(54B)	105.9
H(54A)-C(54)-H(54B)	105.8
C(54)-C(55)-C(56)	127.3(3)
C(54)-C(55)-H(55A)	105.7
C(56)-C(55)-H(55A)	105.6
C(54)-C(55)-H(55B)	104.8
C(56)-C(55)-H(55B)	105.8
H(55A)-C(55)-H(55B)	106.0
C(53)^{i}-C(56)-C(55)	124.6(4)
C(53)^{i}-C(56)-H(56A)	106.2
C(55)-C(56)-H(56A)	106.3
C(53)^{i}-C(56)-H(56B)	105.7
C(55)-C(56)-H(56B)	106.5
H(56A)-C(56)-H(56B)	106.3

Symmetry transformations used to generate equivalent atoms:
(*i*) -x+2,-y+1,-z

Table S9. Anisotropic displacement parameters ($Å^2 x\ 10^4$) for Complex 2. The anisotropic displacement factor exponent takes the form: $-2p^2 [h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ru	145(1)	143(1)	146(1)	4(1)	20(1)	8(1)
Cl(1)	186(2)	190(2)	241(3)	-29(2)	16(2)	-28(2)
Cl(2)	174(2)	174(2)	220(3)	-4(2)	37(2)	-15(2)
P	160(2)	170(3)	196(3)	15(2)	19(2)	13(2)
N(1)	223(9)	160(8)	179(9)	-4(7)	43(7)	27(7)
N(2)	204(9)	159(8)	202(9)	-8(7)	43(7)	31(7)
C(1)	127(9)	162(10)	216(10)	2(8)	22(8)	-35(8)
C(2)	276(12)	166(10)	261(12)	-9(9)	85(10)	26(9)
C(3)	270(11)	194(11)	247(12)	-10(9)	63(9)	53(9)
C(4)	265(11)	149(10)	192(10)	-14(8)	93(9)	31(8)
C(5)	281(11)	174(10)	184(10)	-35(8)	65(9)	-3(9)
C(6)	307(12)	246(12)	200(11)	-13(9)	24(9)	19(9)
C(7)	386(13)	237(11)	225(12)	21(9)	92(10)	-3(10)
C(8)	296(12)	231(11)	276(12)	-12(9)	112(10)	-52(10)
C(9)	236(10)	202(10)	214(11)	-41(8)	75(8)	9(9)
C(10)	303(13)	233(12)	234(12)	-18(9)	5(10)	-38(10)
C(11)	525(18)	382(15)	309(15)	116(12)	57(12)	-60(14)
C(12)	228(11)	255(12)	261(12)	-5(10)	80(9)	-10(10)
C(13)	200(10)	165(10)	194(10)	11(8)	26(8)	68(8)
C(14)	204(10)	171(10)	271(12)	12(8)	18(9)	59(8)
C(15)	262(12)	237(12)	282(12)	-22(9)	-53(10)	63(9)
C(16)	350(13)	263(12)	222(12)	1(9)	10(10)	93(10)
C(17)	299(12)	228(11)	250(12)	61(9)	80(10)	59(9)
C(18)	221(10)	167(10)	250(11)	7(8)	34(9)	64(8)
C(19)	217(11)	249(12)	346(14)	29(10)	-14(10)	1(9)
C(20)	568(19)	399(16)	258(14)	35(11)	-11(13)	103(14)
C(21)	254(12)	236(12)	298(13)	28(10)	57(10)	0(10)
C(22)	185(10)	153(10)	210(10)	-5(8)	9(8)	36(8)
C(23)	282(11)	148(10)	193(11)	6(8)	61(9)	57(8)
C(24)	330(12)	208(11)	222(11)	-1(9)	46(10)	53(9)
C(25)	493(15)	279(12)	167(11)	28(9)	59(10)	85(11)
C(26)	478(15)	268(12)	271(13)	53(10)	190(11)	37(11)
C(27)	356(13)	264(12)	327(13)	43(10)	133(11)	-13(10)
C(28)	286(12)	229(11)	229(11)	18(9)	68(9)	26(9)
C(29)	176(10)	189(10)	202(11)	-3(8)	34(8)	14(8)
C(30)	307(12)	211(11)	208(11)	17(9)	15(9)	74(9)
C(31)	372(14)	291(13)	234(12)	-57(10)	-79(10)	35(10)
C(32)	395(14)	228(12)	339(14)	-78(10)	-7(11)	16(11)
C(33)	256(12)	191(11)	338(13)	-12(9)	5(10)	67(9)
C(34)	201(11)	202(11)	297(12)	6(9)	-3(9)	32(9)
C(35)	173(10)	186(11)	402(13)	-9(9)	85(9)	7(8)
C(36)	306(13)	237(12)	371(14)	77(10)	141(11)	35(10)
C(37)	471(16)	268(14)	637(19)	90(13)	318(15)	12(12)

C(38)	300(14)	218(12)	860(20)	20(13)	322(15)	-25(10)
C(39)	199(12)	291(14)	760(20)	-73(13)	113(13)	1(10)
C(40)	179(11)	298(13)	436(15)	-20(11)	33(10)	24(9)
C(41)	188(10)	216(11)	217(11)	37(8)	-28(8)	13(9)
C(42)	269(12)	257(12)	240(11)	-4(9)	31(9)	-25(10)
C(43)	355(14)	337(14)	226(12)	-39(10)	-23(10)	4(11)
C(44)	432(15)	340(14)	223(12)	60(10)	13(11)	71(11)
C(45)	453(15)	316(14)	282(13)	119(11)	-25(11)	-77(12)
C(46)	340(13)	348(14)	263(13)	94(10)	-40(10)	-102(11)
C(47)	453(16)	392(16)	670(20)	26(14)	263(15)	-75(13)
C(48)	315(13)	569(17)	253(13)	-95(12)	79(10)	-26(12)
C(49)	720(20)	310(16)	1130(30)	26(18)	660(20)	67(15)
C(50)	1060(40)	1740(50)	1050(40)	1150(40)	910(30)	1190(40)
C(51)	380(20)	2840(80)	310(20)	-250(30)	-105(15)	750(40)
C(52)	345(18)	1290(40)	1070(30)	-840(30)	140(20)	-300(20)
C(53)	1500(40)	940(30)	590(30)	-80(20)	-310(30)	-170(30)
C(54)	1320(70)	310(30)	450(40)	10(30)	-50(50)	-110(50)
C(55)	2110(80)	480(30)	240(30)	-90(20)	-180(40)	-440(50)
C(56)	790(40)	610(40)	120(20)	40(20)	50(30)	-530(30)

Table S10. Hydrogen coordinates (x 10^3) and isotropic displacement parameters (Å^{2}x 10^3) for Complex 2.

	x	y	z	U_{iso}
H(2A)	-130(2)	288(2)	303(1)	28
H(2B)	-247(2)	244(1)	300(1)	28
H(3A)	-287(2)	278(1)	221(1)	28
H(3B)	-187(2)	340(2)	224(1)	28
H(6)	35(2)	55(1)	423(1)	30
H(8)	-258(2)	-45(2)	370(1)	31
H(10A)	60(2)	201(2)	322(1)	31
H(10B)	130(2)	146(2)	358(1)	31
H(10C)	63(2)	212(2)	376(1)	31
H(11A)	-38(2)	-63(2)	469(1)	49
H(11B)	-108(2)	-127(2)	439(1)	49
H(11C)	-156(2)	-56(2)	467(1)	49
H(12A)	-367(2)	14(2)	301(1)	29
H(12B)	-298(2)	20(2)	259(1)	29
H(12C)	-339(2)	104(2)	281(1)	29
H(15)	-344(2)	156(2)	55(1)	32
H(17)	-85(2)	321(2)	60(1)	31
H(19A)	-405(2)	101(2)	127(1)	33
H(19B)	-365(2)	145(2)	177(1)	33
H(19C)	-305(2)	67(2)	161(1)	33
H(20A)	-234(2)	201(2)	-25(1)	50
H(20B)	-196(2)	291(2)	-20(1)	50
H(20C)	-298(2)	276(2)	-17(1)	50
H(21A)	-38(2)	366(2)	175(1)	31
H(21B)	30(2)	354(2)	134(1)	31
H(21C)	35(2)	287(2)	175(1)	31
H(22)	-111(2)	21(1)	129(1)	22
H(24)	-108(2)	45(1)	49(1)	30
H(25)	-26(2)	101(2)	-17(1)	37
H(26)	139(2)	176(2)	-4(1)	39
H(27)	225(2)	199(2)	76(1)	37
H(28)	146(2)	142(1)	144(1)	29
H(29)	6(2)	-204(1)	198(1)	23
H(30A)	59(2)	-173(1)	104(1)	29
H(30B)	-44(2)	-136(2)	123(1)	29
H(31A)	-113(2)	-283(2)	132(1)	37
H(31B)	-84(2)	-268(2)	79(1)	37
H(32A)	-11(2)	-404(2)	110(1)	39
H(32B)	85(2)	-344(2)	96(1)	39
H(33A)	137(2)	-401(2)	175(1)	32
H(33B)	32(2)	-372(2)	195(1)	32
H(34A)	202(2)	-257(1)	166(1)	28
H(34B)	179(2)	-272(1)	222(1)	28
H(35)	245(2)	9(2)	201(1)	30
H(36A)	244(2)	-127(2)	129(1)	36
H(36B)	181(2)	-40(2)	119(1)	36

H(37A)	344(2)	38(2)	129(1)	52
H(37B)	343(2)	-30(2)	85(1)	52
H(38A)	451(2)	-128(2)	142(1)	53
H(38B)	513(2)	-40(2)	142(1)	53
H(39A)	450(2)	5(2)	218(1)	49
H(39B)	513(2)	-85(2)	223(1)	49
H(40A)	345(2)	-87(2)	259(1)	37
H(40B)	343(2)	-160(2)	216(1)	37
H(41)	204(2)	-160(1)	278(1)	25
H(42A)	105(2)	-16(2)	315(1)	31
H(42B)	219(2)	-8(2)	301(1)	31
H(43A)	276(2)	-113(2)	365(1)	37
H(43B)	231(2)	-31(2)	388(1)	37
H(44A)	65(2)	-110(2)	390(1)	40
H(44B)	164(2)	-167(2)	417(1)	40
H(45A)	41(2)	-259(2)	362(1)	43
H(45B)	157(2)	-260(2)	346(1)	43
H(46A)	-13(2)	-146(2)	299(1)	39
H(46B)	33(2)	-237(2)	275(1)	39
H(47)	665	721	88	59
H(48)	721	859	115	45
H(49)	686	981	63	80
H(50)	591	958	-19	146
H(51)	542	811	-42	143
H(52)	580	698	11	108
H(53A)[a]	746	566	10	126
H(53B)[a]	844	632	23	126
H(53C)[a]	806	605	-32	126
H(53D)[a]	1225	357	6	126
H(53E)[a]	1190	423	-38	126
H(53F)[a]	1234	460	15	126
H(53G)[a]	782	641	-7	126
H(53H)[a]	774	538	-16	126
H(53I)[a]	817	575	37	126
H(53J)[a]	1262	433	-12	126
H(53K)[a]	1202	393	31	126
H(53L)[a]	1164	366	-25	126
H(54A)[a]	859	457	-13	85
H(54B)[a]	895	483	41	85
H(54C)[a]	1138	543	12	85
H(54D)[a]	1101	517	-42	85
H(55A)[a]	1036	548	19	116
H(55B)[a]	999	516	-34	116
H(55C)[a]	1001	484	34	116
H(55D)[a]	964	451	-19	116
H(56A)[a]	1046	366	-7	61
H(56B)[a]	1088	403	44	61
H(56C)[a]	950	635	8	61
H(56D)[a]	907	599	-44	61

[a] Population: ¼

Figure S13. Crystal Structure of Complex **7**

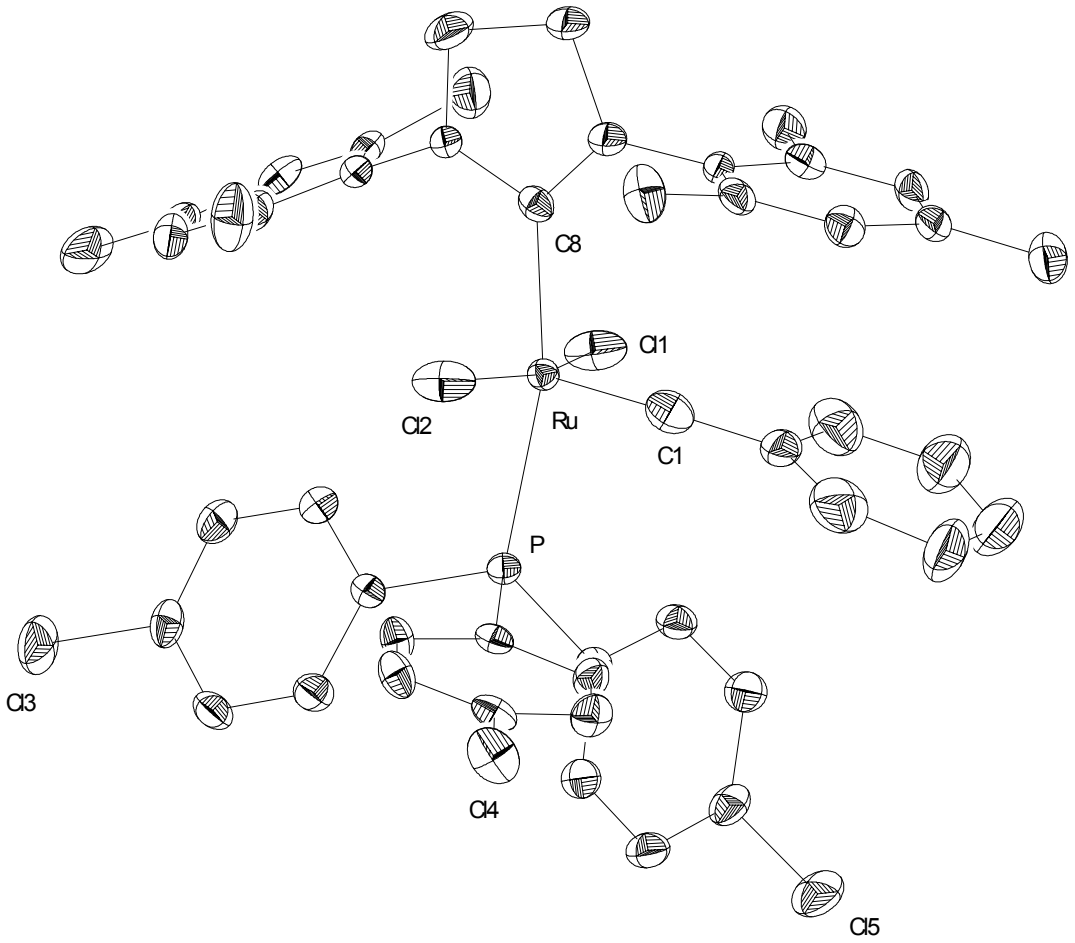


Table S11. Crystal data and structure refinement for Complex 7.

Empirical formula	$C_{46}H_{44}Cl_5N_2PRu \cdot \frac{1}{2}(C_6H_6)$
Formula weight	973.18
Crystallization Solvent	Benzene/pentane
Crystal Habit	Fragment
Crystal size	0.29 x 0.18 x 0.07 mm^3
Crystal color	Dark brown

Data Collection

Type of diffractometer	Bruker SMART 1000
Wavelength	0.71073 Å MoKα
Data Collection Temperature	98(2) K
θ range for 21054 reflections used in lattice determination	2.18 to 28.37°
Unit cell dimensions	a = 12.9550(7) Å b = 13.7527(7) Å β= 101.7540(10)° c = 25.7007(13) Å
Volume	4483.0(4) $Å^3$
Z	4
Crystal system	Monoclinic
Space group	$P2_1/c$
Density (calculated)	1.442 Mg/m^3
F(000)	1996
Data collection program	Bruker SMART v5.054
θ range for data collection	1.61 to 28.49°
Completeness to θ = 28.49°	94.6 %
Index ranges	$-17 \le h \le 17$, $-18 \le k \le 18$, $-34 \le l \le 34$
Data collection scan type	ω scans at 7 ϕ settings
Data reduction program	Bruker SAINT v6.22
Reflections collected	102600
Independent reflections	10763 [R_{int}= 0.0974]
Absorption coefficient	0.720 mm^{-1}
Absorption correction	None
Max. and min. transmission	0.9486 and 0.8189

Table S11 (cont.)

Structure solution and Refinement

Structure solution program	SHELXS-97 (Sheldrick, 1990)
Primary solution method	Direct methods
Secondary solution method	Difference Fourier map
Hydrogen placement	Geometric positions
Structure refinement program	SHELXL-97 (Sheldrick, 1997)
Refinement method	Full matrix least-squares on F^2
Data / restraints / parameters	10763 / 0 / 529
Treatment of hydrogen atoms	Riding
Goodness-of-fit on F^2	1.869
Final R indices [I>2σ(I), 7096 reflections]	R1 = 0.0552, *w*R2 = 0.0803
R indices (all data)	R1 = 0.0969, *w*R2 = 0.0839
Type of weighting scheme used	Sigma
Weighting scheme used	$w=1/\sigma^2(Fo^2)$
Max shift/error	0.048
Average shift/error	0.000
Largest diff. peak and hole	2.173 and -1.352 e.Å^{-3}

Special Refinement Details

There are three peaks in the final difference electron density Fourier map that are in excess of 1 e$^-$/Å^3. two of these are within an angstrom of a chlorine atom and may be attributed to absorption. The third strongest peak lies approx. 1.8Å from Ru and approx. 1.1Å from C1; part of a series of peaks that suggest disorder in the orientation of the carbene ligand. It was not possible to adequately model disorder at this site.

Refinement of F^2 against ALL reflections. The weighted R-factor (*w*R) and goodness of fit (S) are based on F^2, conventional R-factors (R) are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Table S12. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for Complex 7. U(eq) is defined as the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
Ru(1)	2590(1)	3202(1)	2952(1)	15(1)
Cl(1)	1023(1)	4031(1)	3030(1)	35(1)
Cl(2)	3937(1)	2359(1)	2631(1)	36(1)
Cl(3)	2349(1)	6562(1)	615(1)	43(1)
Cl(4)	8331(1)	3339(1)	3381(1)	36(1)
Cl(5)	3315(1)	8298(1)	4392(1)	40(1)
P(1)	3566(1)	4667(1)	2902(1)	15(1)
N(1)	1267(2)	1621(2)	2323(1)	21(1)
N(2)	1824(2)	1128(2)	3135(1)	23(1)
C(1)	3355(4)	3020(3)	3630(2)	51(1)
C(2)	3386(3)	3355(3)	4157(2)	27(1)
C(3)	2485(4)	3738(3)	4315(2)	48(1)
C(4)	2533(4)	4071(3)	4828(2)	52(1)
C(5)	3513(4)	4046(3)	5190(2)	54(1)
C(6)	4418(5)	3680(3)	5050(2)	57(2)
C(7)	4320(4)	3299(3)	4532(2)	51(1)
C(8)	1786(3)	1898(3)	2808(1)	19(1)
C(9)	1005(4)	583(3)	2291(2)	40(1)
C(10)	1256(3)	272(3)	2872(1)	32(1)
C(11)	916(3)	2233(3)	1872(1)	20(1)
C(12)	-68(3)	2675(3)	1817(1)	23(1)
C(13)	-423(3)	3261(3)	1377(1)	27(1)
C(14)	161(3)	3392(3)	984(1)	28(1)
C(15)	1096(3)	2895(3)	1036(1)	31(1)
C(16)	1495(3)	2296(3)	1470(1)	25(1)
C(17)	-753(3)	2507(3)	2214(2)	37(1)
C(18)	-237(3)	4027(3)	509(2)	45(1)
C(19)	2460(3)	1686(3)	1463(2)	45(1)
C(20)	2223(3)	1112(2)	3700(1)	20(1)
C(21)	1595(3)	1458(3)	4037(1)	22(1)
C(22)	2004(3)	1441(3)	4580(1)	25(1)
C(23)	3001(3)	1089(3)	4791(1)	23(1)
C(24)	3600(3)	730(3)	4441(1)	25(1)
C(25)	3221(3)	714(3)	3894(2)	23(1)
C(26)	516(3)	1866(3)	3821(1)	30(1)
C(27)	3444(3)	1108(3)	5377(1)	33(1)
C(28)	3856(3)	269(3)	3529(2)	35(1)
C(29)	3235(3)	5202(2)	2238(1)	16(1)
C(30)	2301(3)	4942(3)	1895(1)	23(1)
C(31)	2027(3)	5360(3)	1396(2)	29(1)
C(32)	2678(3)	6039(3)	1248(1)	25(1)
C(33)	3608(3)	6316(3)	1573(1)	25(1)
C(34)	3874(3)	5887(3)	2066(1)	24(1)
C(35)	4979(3)	4438(2)	3016(1)	17(1)
C(36)	5471(3)	4126(2)	2614(1)	21(1)

C(37)	6496(3)	3795(3)	2726(2)	26(1)
C(38)	7049(3)	3782(3)	3244(2)	23(1)
C(39)	6591(3)	4095(3)	3652(2)	25(1)
C(40)	5560(3)	4417(3)	3536(1)	23(1)
C(41)	3503(3)	5721(2)	3332(1)	16(1)
C(42)	2726(3)	5779(3)	3629(1)	22(1)
C(43)	2667(3)	6565(3)	3956(1)	28(1)
C(44)	3379(3)	7310(3)	3974(1)	26(1)
C(45)	4154(3)	7290(3)	3681(1)	26(1)
C(46)	4217(3)	6486(3)	3365(1)	23(1)
C(51)	10183(4)	5782(4)	4684(2)	65(2)
C(52)	9770(4)	4934(5)	4448(2)	72(2)
C(53)	9587(4)	4138(4)	4778(3)	66(2)

Table S13. Selected bond lengths [Å] and angles [°] for Complex 7.

Ru(1)-C(1)	1.836(4)	C(1)-Ru(1)-C(8)	101.94(15)
Ru(1)-C(8)	2.070(4)	C(1)-Ru(1)-Cl(1)	107.01(16)
Ru(1)-Cl(1)	2.3713(10)	C(8)-Ru(1)-Cl(1)	91.35(9)
Ru(1)-Cl(2)	2.3803(10)	C(1)-Ru(1)-Cl(2)	88.28(16)
Ru(1)-P(1)	2.3961(10)	C(8)-Ru(1)-Cl(2)	83.84(9)
		Cl(1)-Ru(1)-Cl(2)	164.64(4)
		C(1)-Ru(1)-P(1)	88.68(12)
		C(8)-Ru(1)-P(1)	166.12(9)
		Cl(1)-Ru(1)-P(1)	94.07(3)
		Cl(2)-Ru(1)-P(1)	87.62(3)

Table S14. Bond lengths [Å] and angles [°] for Complex 7.

Ru(1)-C(1)	1.836(4)	C(18)-H(18B)	0.9800
Ru(1)-C(8)	2.070(4)	C(18)-H(18C)	0.9800
Ru(1)-Cl(1)	2.3713(10)	C(19)-H(19A)	0.9800
Ru(1)-Cl(2)	2.3803(10)	C(19)-H(19B)	0.9800
Ru(1)-P(1)	2.3961(10)	C(19)-H(19C)	0.9800
Cl(3)-C(32)	1.748(4)	C(20)-C(21)	1.389(5)
Cl(4)-C(38)	1.736(4)	C(20)-C(25)	1.399(5)
Cl(5)-C(44)	1.745(4)	C(21)-C(22)	1.386(5)
P(1)-C(35)	1.822(3)	C(21)-C(26)	1.503(5)
P(1)-C(29)	1.827(3)	C(22)-C(23)	1.383(5)
P(1)-C(41)	1.835(3)	C(22)-H(22)	0.9500
N(1)-C(8)	1.345(4)	C(23)-C(24)	1.392(5)
N(1)-C(11)	1.429(4)	C(23)-C(27)	1.498(5)
N(1)-C(9)	1.465(4)	C(24)-C(25)	1.392(5)
N(2)-C(8)	1.347(4)	C(24)-H(24)	0.9500
N(2)-C(20)	1.439(4)	C(25)-C(28)	1.498(5)
N(2)-C(10)	1.478(4)	C(26)-H(26A)	0.9800
C(1)-C(2)	1.426(5)	C(26)-H(26B)	0.9800
C(1)-H(1)	0.9500	C(26)-H(26C)	0.9800
C(2)-C(7)	1.387(5)	C(27)-H(27A)	0.9800
C(2)-C(3)	1.413(5)	C(27)-H(27B)	0.9800
C(3)-C(4)	1.386(6)	C(27)-H(27C)	0.9800
C(3)-H(3)	0.9500	C(28)-H(28A)	0.9800
C(4)-C(5)	1.412(6)	C(28)-H(28B)	0.9800
C(4)-H(4)	0.9500	C(28)-H(28C)	0.9800
C(5)-C(6)	1.389(6)	C(29)-C(34)	1.385(4)
C(5)-H(5)	0.9500	C(29)-C(30)	1.390(4)
C(6)-C(7)	1.412(6)	C(30)-C(31)	1.384(5)
C(6)-H(6)	0.9500	C(30)-H(30)	0.9500
C(7)-H(7)	0.9500	C(31)-C(32)	1.365(5)
C(9)-C(10)	1.523(5)	C(31)-H(31)	0.9500
C(9)-H(9A)	0.9900	C(32)-C(33)	1.373(5)
C(9)-H(9B)	0.9900	C(33)-C(34)	1.377(5)
C(10)-H(10A)	0.9900	C(33)-H(33)	0.9500
C(10)-H(10B)	0.9900	C(34)-H(34)	0.9500
C(11)-C(12)	1.393(5)	C(35)-C(36)	1.388(4)
C(11)-C(16)	1.399(5)	C(35)-C(40)	1.394(5)
C(12)-C(13)	1.390(5)	C(36)-C(37)	1.377(5)
C(12)-C(17)	1.500(5)	C(36)-H(36)	0.9500
C(13)-C(14)	1.392(5)	C(37)-C(38)	1.377(5)
C(13)-H(13)	0.9500	C(37)-H(37)	0.9500
C(14)-C(15)	1.373(5)	C(38)-C(39)	1.376(5)
C(14)-C(18)	1.505(5)	C(39)-C(40)	1.381(5)
C(15)-C(16)	1.397(5)	C(39)-H(39)	0.9500
C(15)-H(15)	0.9500	C(40)-H(40)	0.9500
C(16)-C(19)	1.508(5)	C(41)-C(42)	1.382(4)
C(17)-H(17A)	0.9800	C(41)-C(46)	1.392(4)
C(17)-H(17B)	0.9800	C(42)-C(43)	1.381(5)
C(17)-H(17C)	0.9800	C(42)-H(42)	0.9500
C(18)-H(18A)	0.9800	C(43)-C(44)	1.373(5)

C(43)-H(43)	0.9500	C(7)-C(6)-H(6)	121.3
C(44)-C(45)	1.372(5)	C(2)-C(7)-C(6)	122.2(5)
C(45)-C(46)	1.385(5)	C(2)-C(7)-H(7)	118.9
C(45)-H(45)	0.9500	C(6)-C(7)-H(7)	118.9
C(46)-H(46)	0.9500	N(1)-C(8)-N(2)	107.7(3)
C(51)-C(53)#1	1.358(7)	N(1)-C(8)-Ru(1)	123.4(2)
C(51)-C(52)	1.373(7)	N(2)-C(8)-Ru(1)	128.0(2)
C(51)-H(51)	0.9500	N(1)-C(9)-C(10)	102.7(3)
C(52)-C(53)	1.435(7)	N(1)-C(9)-H(9A)	111.2
C(52)-H(52)	0.9500	C(10)-C(9)-H(9A)	111.2
C(53)-C(51)#1	1.358(7)	N(1)-C(9)-H(9B)	111.2
C(53)-H(53)	0.9500	C(10)-C(9)-H(9B)	111.2
		H(9A)-C(9)-H(9B)	109.1
C(1)-Ru(1)-C(8)	101.94(15)	N(2)-C(10)-C(9)	102.2(3)
C(1)-Ru(1)-Cl(1)	107.01(16)	N(2)-C(10)-H(10A)	111.3
C(8)-Ru(1)-Cl(1)	91.35(9)	C(9)-C(10)-H(10A)	111.3
C(1)-Ru(1)-Cl(2)	88.28(16)	N(2)-C(10)-H(10B)	111.3
C(8)-Ru(1)-Cl(2)	83.84(9)	C(9)-C(10)-H(10B)	111.3
Cl(1)-Ru(1)-Cl(2)	164.64(4)	H(10A)-C(10)-H(10B)	109.2
C(1)-Ru(1)-P(1)	88.68(12)	C(12)-C(11)-C(16)	121.1(3)
C(8)-Ru(1)-P(1)	166.12(9)	C(12)-C(11)-N(1)	118.2(3)
Cl(1)-Ru(1)-P(1)	94.07(3)	C(16)-C(11)-N(1)	120.3(3)
Cl(2)-Ru(1)-P(1)	87.62(3)	C(13)-C(12)-C(11)	118.7(3)
C(35)-P(1)-C(29)	104.87(16)	C(13)-C(12)-C(17)	120.0(3)
C(35)-P(1)-C(41)	101.89(16)	C(11)-C(12)-C(17)	121.3(3)
C(29)-P(1)-C(41)	102.38(15)	C(12)-C(13)-C(14)	121.8(4)
C(35)-P(1)-Ru(1)	111.72(11)	C(12)-C(13)-H(13)	119.1
C(29)-P(1)-Ru(1)	111.28(12)	C(14)-C(13)-H(13)	119.1
C(41)-P(1)-Ru(1)	122.87(12)	C(15)-C(14)-C(13)	117.6(4)
C(8)-N(1)-C(11)	126.9(3)	C(15)-C(14)-C(18)	121.2(4)
C(8)-N(1)-C(9)	113.2(3)	C(13)-C(14)-C(18)	121.2(4)
C(11)-N(1)-C(9)	119.8(3)	C(14)-C(15)-C(16)	123.2(4)
C(8)-N(2)-C(20)	127.0(3)	C(14)-C(15)-H(15)	118.4
C(8)-N(2)-C(10)	112.9(3)	C(16)-C(15)-H(15)	118.4
C(20)-N(2)-C(10)	119.6(3)	C(11)-C(16)-C(15)	117.3(4)
C(2)-C(1)-Ru(1)	139.7(4)	C(11)-C(16)-C(19)	123.0(3)
C(2)-C(1)-H(1)	110.2	C(15)-C(16)-C(19)	119.5(3)
Ru(1)-C(1)-H(1)	110.2	C(12)-C(17)-H(17A)	109.5
C(7)-C(2)-C(3)	118.5(4)	C(12)-C(17)-H(17B)	109.5
C(7)-C(2)-C(1)	119.6(4)	H(17A)-C(17)-H(17B)	109.5
C(3)-C(2)-C(1)	121.9(4)	C(12)-C(17)-H(17C)	109.5
C(4)-C(3)-C(2)	121.1(5)	H(17A)-C(17)-H(17C)	109.5
C(4)-C(3)-H(3)	119.5	H(17B)-C(17)-H(17C)	109.5
C(2)-C(3)-H(3)	119.5	C(14)-C(18)-H(18A)	109.5
C(3)-C(4)-C(5)	118.6(5)	C(14)-C(18)-H(18B)	109.5
C(3)-C(4)-H(4)	120.7	H(18A)-C(18)-H(18B)	109.5
C(5)-C(4)-H(4)	120.7	C(14)-C(18)-H(18C)	109.5
C(6)-C(5)-C(4)	122.1(5)	H(18A)-C(18)-H(18C)	109.5
C(6)-C(5)-H(5)	118.9	H(18B)-C(18)-H(18C)	109.5
C(4)-C(5)-H(5)	118.9	C(16)-C(19)-H(19A)	109.5
C(5)-C(6)-C(7)	117.4(5)	C(16)-C(19)-H(19B)	109.5
C(5)-C(6)-H(6)	121.3	H(19A)-C(19)-H(19B)	109.5

C(16)-C(19)-H(19C)	109.5	C(32)-C(33)-H(33)	121.1
H(19A)-C(19)-H(19C)	109.5	C(34)-C(33)-H(33)	121.1
H(19B)-C(19)-H(19C)	109.5	C(33)-C(34)-C(29)	122.1(3)
C(21)-C(20)-C(25)	121.9(3)	C(33)-C(34)-H(34)	119.0
C(21)-C(20)-N(2)	119.3(3)	C(29)-C(34)-H(34)	119.0
C(25)-C(20)-N(2)	118.8(3)	C(36)-C(35)-C(40)	117.8(3)
C(20)-C(21)-C(22)	118.0(3)	C(36)-C(35)-P(1)	122.2(3)
C(20)-C(21)-C(26)	121.0(3)	C(40)-C(35)-P(1)	119.1(3)
C(22)-C(21)-C(26)	121.0(3)	C(37)-C(36)-C(35)	121.1(3)
C(23)-C(22)-C(21)	122.4(3)	C(37)-C(36)-H(36)	119.5
C(23)-C(22)-H(22)	118.8	C(35)-C(36)-H(36)	119.5
C(21)-C(22)-H(22)	118.8	C(38)-C(37)-C(36)	119.7(3)
C(22)-C(23)-C(24)	118.0(3)	C(38)-C(37)-H(37)	120.1
C(22)-C(23)-C(27)	121.6(3)	C(36)-C(37)-H(37)	120.1
C(24)-C(23)-C(27)	120.4(3)	C(37)-C(38)-C(39)	120.9(3)
C(23)-C(24)-C(25)	122.0(4)	C(37)-C(38)-Cl(4)	119.2(3)
C(23)-C(24)-H(24)	119.0	C(39)-C(38)-Cl(4)	119.9(3)
C(25)-C(24)-H(24)	119.0	C(38)-C(39)-C(40)	118.9(3)
C(24)-C(25)-C(20)	117.6(3)	C(38)-C(39)-H(39)	120.5
C(24)-C(25)-C(28)	120.9(3)	C(40)-C(39)-H(39)	120.5
C(20)-C(25)-C(28)	121.5(3)	C(39)-C(40)-C(35)	121.6(3)
C(21)-C(26)-H(26A)	109.5	C(39)-C(40)-H(40)	119.2
C(21)-C(26)-H(26B)	109.5	C(35)-C(40)-H(40)	119.2
H(26A)-C(26)-H(26B)	109.5	C(42)-C(41)-C(46)	118.2(3)
C(21)-C(26)-H(26C)	109.5	C(42)-C(41)-P(1)	120.3(3)
H(26A)-C(26)-H(26C)	109.5	C(46)-C(41)-P(1)	121.5(3)
H(26B)-C(26)-H(26C)	109.5	C(43)-C(42)-C(41)	121.2(3)
C(23)-C(27)-H(27A)	109.5	C(43)-C(42)-H(42)	119.4
C(23)-C(27)-H(27B)	109.5	C(41)-C(42)-H(42)	119.4
H(27A)-C(27)-H(27B)	109.5	C(44)-C(43)-C(42)	118.9(4)
C(23)-C(27)-H(27C)	109.5	C(44)-C(43)-H(43)	120.5
H(27A)-C(27)-H(27C)	109.5	C(42)-C(43)-H(43)	120.5
H(27B)-C(27)-H(27C)	109.5	C(45)-C(44)-C(43)	121.9(3)
C(25)-C(28)-H(28A)	109.5	C(45)-C(44)-Cl(5)	119.0(3)
C(25)-C(28)-H(28B)	109.5	C(43)-C(44)-Cl(5)	119.1(3)
H(28A)-C(28)-H(28B)	109.5	C(44)-C(45)-C(46)	118.4(4)
C(25)-C(28)-H(28C)	109.5	C(44)-C(45)-H(45)	120.8
H(28A)-C(28)-H(28C)	109.5	C(46)-C(45)-H(45)	120.8
H(28B)-C(28)-H(28C)	109.5	C(45)-C(46)-C(41)	121.3(3)
C(34)-C(29)-C(30)	118.2(3)	C(45)-C(46)-H(46)	119.3
C(34)-C(29)-P(1)	122.0(3)	C(41)-C(46)-H(46)	119.3
C(30)-C(29)-P(1)	119.7(3)	C(53)#1-C(51)-C(52)	120.3(5)
C(31)-C(30)-C(29)	120.4(4)	C(53)#1-C(51)-H(51)	119.8
C(31)-C(30)-H(30)	119.8	C(52)-C(51)-H(51)	119.8
C(29)-C(30)-H(30)	119.8	C(51)-C(52)-C(53)	118.9(5)
C(32)-C(31)-C(30)	119.2(4)	C(51)-C(52)-H(52)	120.6
C(32)-C(31)-H(31)	120.4	C(53)-C(52)-H(52)	120.6
C(30)-C(31)-H(31)	120.4	C(51)#1-C(53)-C(52)	120.8(5)
C(31)-C(32)-C(33)	122.3(3)	C(51)#1-C(53)-H(53)	119.6
C(31)-C(32)-Cl(3)	119.6(3)	C(52)-C(53)-H(53)	119.6
C(33)-C(32)-Cl(3)	118.0(3)		
C(32)-C(33)-C(34)	117.8(3)		

Symmetry transformations used to generate equivalent atoms:
#1 -x+2,-y+1,-z+1

Table S15. Anisotropic displacement parameters ($Å^2 x 10^4$) for Complex 7. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ru(1)	146(2)	157(2)	158(2)	-1(1)	31(1)	-3(2)
Cl(1)	172(5)	271(6)	609(7)	-126(5)	119(5)	7(4)
Cl(2)	234(6)	226(6)	638(8)	-94(5)	149(5)	23(5)
Cl(3)	577(8)	457(7)	198(5)	76(5)	-22(5)	28(6)
Cl(4)	200(5)	461(7)	422(6)	120(5)	79(5)	108(5)
Cl(5)	487(7)	322(6)	424(6)	-185(5)	140(5)	-54(6)
P(1)	135(5)	155(5)	171(5)	-2(4)	27(4)	0(4)
N(1)	301(19)	186(18)	156(16)	-13(13)	52(14)	-77(15)
N(2)	290(20)	170(17)	221(18)	-4(14)	42(15)	-50(15)
C(1)	860(40)	310(30)	360(30)	60(20)	130(30)	-240(30)
C(2)	330(20)	230(20)	240(20)	25(18)	6(19)	-60(20)
C(3)	570(30)	410(30)	480(30)	60(20)	180(30)	30(30)
C(4)	620(40)	500(30)	420(30)	-90(30)	90(30)	-10(30)
C(5)	730(40)	490(30)	350(30)	-100(20)	-10(30)	-70(30)
C(6)	830(40)	560(30)	250(30)	-50(20)	-20(30)	-50(30)
C(7)	550(30)	460(30)	480(30)	160(30)	10(20)	-40(30)
C(8)	180(20)	180(20)	220(20)	8(17)	88(16)	13(17)
C(9)	630(30)	220(20)	290(20)	-25(19)	-40(20)	-150(20)
C(10)	480(30)	180(20)	280(20)	-12(18)	50(20)	-130(20)
C(11)	250(20)	190(20)	150(20)	-9(16)	22(17)	-55(17)
C(12)	250(20)	270(20)	180(20)	-85(17)	44(18)	-72(18)
C(13)	240(20)	280(20)	240(20)	-89(19)	-44(17)	-20(20)
C(14)	330(20)	280(20)	180(20)	-2(17)	-50(18)	-70(20)
C(15)	330(30)	420(30)	180(20)	-27(19)	58(19)	-70(20)
C(16)	220(20)	330(20)	170(20)	-39(18)	4(17)	-39(19)
C(17)	320(30)	520(30)	270(20)	-10(20)	80(20)	-50(20)
C(18)	490(30)	450(30)	300(30)	60(20)	-180(20)	-110(20)
C(19)	360(30)	720(40)	280(20)	-20(20)	90(20)	150(30)
C(20)	320(20)	131(19)	135(19)	6(15)	26(17)	-51(17)
C(21)	210(20)	200(20)	260(20)	37(17)	56(18)	-18(17)
C(22)	320(20)	240(20)	230(20)	-25(17)	167(19)	-11(18)
C(23)	310(20)	190(20)	210(20)	13(17)	83(18)	-35(18)
C(24)	300(20)	200(20)	240(20)	44(17)	41(19)	29(18)
C(25)	330(20)	150(20)	240(20)	33(17)	113(19)	-14(18)
C(26)	240(20)	380(20)	300(20)	0(20)	81(18)	-20(20)
C(27)	410(30)	350(30)	240(20)	38(19)	90(20)	30(20)
C(28)	440(30)	320(30)	310(20)	50(20)	150(20)	150(20)
C(29)	150(20)	150(20)	190(20)	6(16)	58(16)	17(16)
C(30)	240(20)	240(20)	210(20)	-21(17)	25(18)	-32(18)
C(31)	270(20)	350(20)	210(20)	-22(19)	-27(18)	-20(20)
C(32)	330(20)	240(20)	160(20)	20(17)	17(18)	85(19)
C(33)	260(20)	260(20)	250(20)	69(18)	63(18)	-47(18)
C(34)	200(20)	270(20)	230(20)	45(18)	-6(17)	-33(18)
C(35)	160(20)	126(19)	240(20)	18(16)	67(17)	-6(16)
C(36)	190(20)	270(20)	180(20)	54(17)	47(17)	52(18)

C(37)	260(20)	290(20)	250(20)	37(18)	149(19)	56(19)
C(38)	160(20)	200(20)	330(20)	69(18)	89(18)	3(17)
C(39)	180(20)	310(20)	240(20)	6(18)	-15(18)	21(18)
C(40)	210(20)	290(20)	200(20)	-48(17)	67(17)	-13(18)
C(41)	160(20)	140(19)	180(20)	26(15)	3(16)	16(16)
C(42)	250(20)	170(20)	260(20)	-2(17)	71(18)	-21(17)
C(43)	290(20)	260(20)	300(20)	-53(18)	121(19)	-26(19)
C(44)	330(20)	200(20)	250(20)	-67(17)	39(19)	18(19)
C(45)	300(20)	210(20)	280(20)	-23(18)	33(19)	-51(19)
C(46)	220(20)	240(20)	250(20)	-36(17)	86(18)	2(17)
C(51)	560(40)	590(40)	740(40)	190(30)	40(30)	70(30)
C(52)	710(40)	750(50)	580(40)	-40(40)	-140(30)	110(40)
C(53)	500(40)	630(40)	800(40)	-140(40)	-20(30)	20(30)

Table S16. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for Complex 7.

	x	y	z	U_{iso}
H(1)	3900	2559	3627	61
H(3)	1836	3769	4065	57
H(4)	1920	4310	4935	62
H(5)	3554	4286	5540	65
H(6)	5077	3687	5293	68
H(7)	4913	2993	4437	61
H(9A)	1442	225	2081	48
H(9B)	251	480	2131	48
H(10A)	604	143	3005	38
H(10B)	1707	-316	2923	38
H(13)	-1083	3582	1343	32
H(15)	1490	2962	765	37
H(17A)	-1439	2818	2089	55
H(17B)	-414	2787	2557	55
H(17C)	-852	1807	2256	55
H(18A)	324	4472	456	67
H(18B)	-844	4404	568	67
H(18C)	-449	3620	192	67
H(19A)	2698	1383	1812	68
H(19B)	3022	2099	1381	68
H(19C)	2286	1179	1191	68
H(22)	1584	1679	4815	30
H(24)	4288	489	4580	30
H(26A)	583	2475	3633	46
H(26B)	155	1990	4114	46
H(26C)	108	1397	3574	46
H(27A)	4140	798	5449	49
H(27B)	2972	754	5563	49
H(27C)	3510	1783	5501	49
H(28A)	3577	-378	3419	52
H(28B)	4593	213	3714	52
H(28C)	3812	682	3214	52
H(30)	1848	4475	2004	28
H(31)	1394	5176	1160	35
H(33)	4053	6787	1461	30
H(34)	4516	6068	2296	29
H(36)	5095	4140	2256	26
H(37)	6820	3576	2447	31
H(39)	6978	4090	4008	30
H(40)	5239	4630	3817	27
H(42)	2225	5269	3607	27
H(43)	2142	6589	4166	33
H(45)	4635	7815	3695	32
H(46)	4760	6455	3166	28
H(51)	10309	6315	4470	77
H(52)	9608	4874	4071	87
H(53)	9301	3547	4619	80

Figure S14. Crystal Structure of Complex **9**

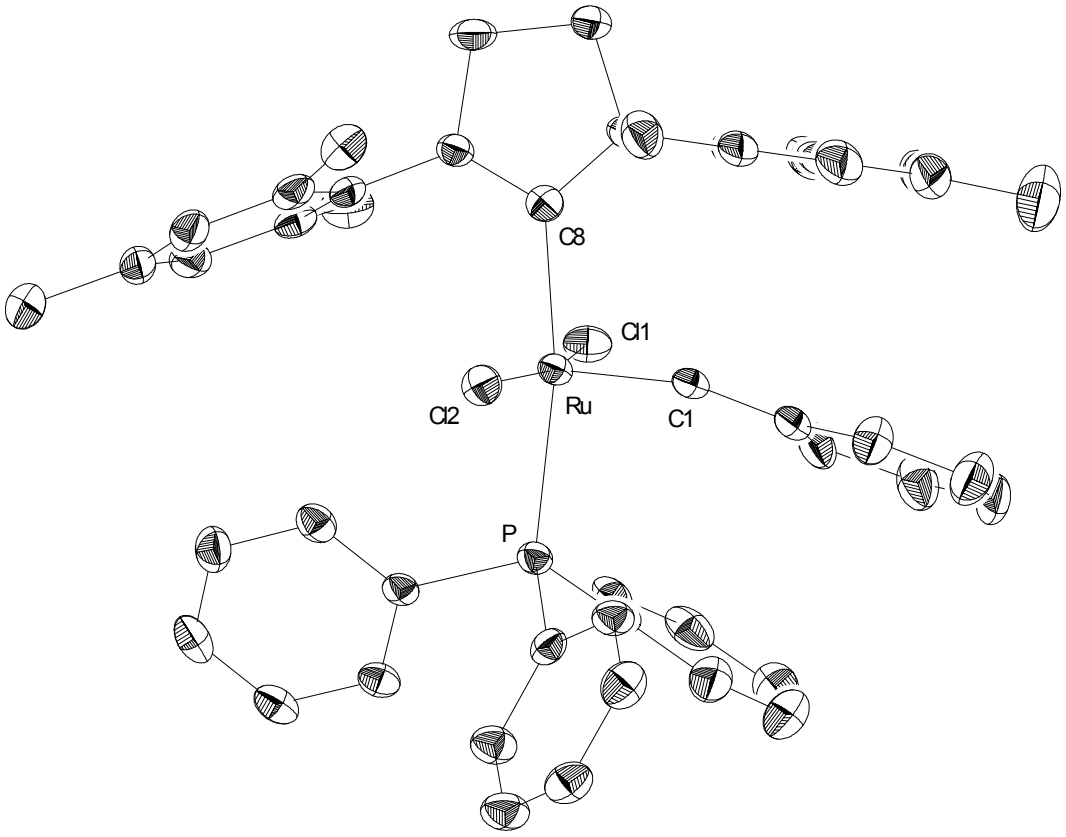


Table S17. Crystal data and structure refinement for Complex 9.

Empirical formula	$C_{46}H_{47}Cl_2N_2PRu \bullet 1\ 1/6(C_6H_6)$
Formula weight	921.92
Crystallization Solvent	Benzene
Crystal Habit	Plates
Crystal size	0.26 x 0.25 x 0.11 mm^3
Crystal color	Pale Brown

Data Collection

Preliminary Photos	Rotation	
Type of diffractometer	CCD area detector	
Wavelength	0.71073 Å MoKα	
Data Collection Temperature	98(2) K	
θ range for 34954 reflections used in lattice determination	2.18 to 28.67°	
Unit cell dimensions	a = 23.6408(7) Å b = 23.6408(7) Å c = 45.2398(19) Å	α= 90° β= 90° γ = 120°
Volume	21896.5(13) $Å^3$	
Z	18	
Crystal system	Rhombohedral	
Space group	R-3 (Hexagonal setting)	
Density (calculated)	1.258 Mg/m^3	
F(000)	8622	
θ range for data collection	1.34 to 28.81°	
Completeness to θ = 28.81°	93.8 %	
Index ranges	$-30 \le h \le 31$, $-30 \le k \le 30$, $-60 \le l \le 58$	
Data collection scan type	ω scans at 5 ϕ settings	
Reflections collected	110902	
Independent reflections	11939 [R_{int}= 0.0743]	
Absorption coefficient	0.500 mm^{-1}	
Absorption correction	None	
Max. and min. transmission (theory)	0.9465 and 0.8813	

Table S17 (cont.)

Structure solution and Refinement

Structure solution program	SHELXS-97 (Sheldrick, 1990)
Primary solution method	Direct methods
Secondary solution method	Difference Fourier map
Hydrogen placement	Geometric positions
Structure refinement program	SHELXL-97 (Sheldrick, 1997)
Refinement method	Full matrix least-squares on F^2
Data / restraints / parameters	11939 / 7 / 505
Treatment of hydrogen atoms	Riding
Goodness-of-fit on F^2	3.793
Final R indices [I>2σ(I), 8768 reflections]	R1 = 0.0552, *w*R2 = 0.1348
R indices (all data)	R1 = 0.0804, *w*R2 = 0.1364
Type of weighting scheme used	Sigma
Weighting scheme used	$w=1/\sigma^2(Fo^2)$
Max shift/error	0.155
Average shift/error	0.001
Largest diff. peak and hole	2.084 and -0.830 e.Å^{-3}

Special Refinement Details

This crystal contains a significant amount of solvent of crystallization (benzene) in both well defined and ill defined regions of the lattice. Equivalent reflections in the data set merge well (R_{merge}=0.07) but the model does not refine well against the data, due to the inclusion of poorly defined solvent in the lattice. The lattice contains one benzene sitting on a 3-fold axis (C51 and C52) and one other benzene sitting on a 3-bar symmetry site (C61). These solvents are well defined, however, one other site near a 3-fold is poorly defined. This site contains three disordered solvents (C71-C76, C81-C82, and C91-C96). The presence of any one of these precludes the presence of the other two. Additionally, H95 sits on the 3-fold axis so C91-C96 is restrained to one-third or less of its possible presence.

Refinement of F^2 against ALL reflections. The weighted R-factor (*w*R) and goodness of fit (S) are based on F^2, conventional R-factors (R) are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Table S18. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for Complex 9. U(eq) the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}	Occ
Ru	89(1)	3228(1)	1151(1)	19(1)	1
Cl(1)	-1047(1)	2670(1)	1040(1)	27(1)	1
Cl(2)	1147(1)	3688(1)	1373(1)	26(1)	1
P	168(1)	2312(1)	973(1)	20(1)	1
N(1)	-364(4)	3770(4)	1647(2)	22(2)	1
N(2)	-203(4)	4352(4)	1251(2)	26(2)	1
C(1)	461(5)	3717(5)	815(2)	22(2)	1
C(2)	302(5)	3648(5)	502(2)	25(2)	1
C(3)	-300(5)	3195(5)	381(2)	33(3)	1
C(4)	-404(6)	3170(6)	77(2)	40(3)	1
C(5)	87(7)	3591(6)	-106(2)	44(3)	1
C(6)	692(6)	4045(6)	6(3)	42(3)	1
C(7)	792(5)	4072(5)	306(2)	33(3)	1
C(8)	-133(5)	3868(5)	1370(2)	21(2)	1
C(9)	-631(5)	4197(5)	1731(2)	30(3)	1
C(10)	-502(6)	4613(5)	1456(2)	33(3)	1
C(11)	-295(5)	3368(5)	1869(2)	21(2)	1
C(12)	287(5)	3631(5)	2035(2)	26(2)	1
C(13)	338(5)	3239(5)	2251(2)	29(3)	1
C(14)	-166(5)	2617(5)	2310(2)	29(3)	1
C(15)	-739(5)	2381(5)	2154(2)	29(3)	1
C(16)	-826(5)	2750(5)	1933(2)	24(2)	1
C(17)	825(5)	4323(5)	1995(2)	30(3)	1
C(18)	-100(6)	2205(6)	2544(2)	43(3)	1
C(19)	-1486(5)	2503(5)	1787(2)	34(3)	1
C(20)	111(5)	4719(5)	988(2)	27(2)	1
C(21)	764(6)	5175(5)	1002(2)	30(3)	1
C(22)	1071(6)	5542(5)	749(3)	39(3)	1
C(23)	724(7)	5452(6)	485(3)	41(3)	1
C(24)	63(6)	5006(5)	486(2)	36(3)	1
C(25)	-255(6)	4631(5)	733(2)	31(3)	1
C(26)	1158(5)	5285(5)	1281(2)	35(3)	1
C(27)	1077(7)	5825(6)	207(3)	57(4)	1
C(28)	-979(6)	4128(5)	720(2)	38(3)	1
C(29)	-112(4)	1666(5)	1255(2)	19(2)	1
C(30)	-36(5)	1848(5)	1552(2)	25(2)	1
C(31)	-200(5)	1376(5)	1769(2)	30(3)	1
C(32)	-431(5)	739(5)	1694(2)	31(3)	1
C(33)	-510(5)	556(5)	1403(2)	27(2)	1
C(34)	-358(4)	1011(5)	1184(2)	24(2)	1
C(35)	982(5)	2452(5)	874(2)	22(2)	1
C(36)	1136(5)	1950(5)	899(2)	29(3)	1
C(37)	1747(5)	2058(5)	822(2)	32(3)	1
C(38)	2216(5)	2656(5)	723(2)	31(3)	1
C(39)	2070(5)	3161(5)	698(2)	33(3)	1
C(40)	1461(5)	3059(5)	773(2)	25(2)	1

C(41)	-323(5)	1891(5)	651(2)	23(2)	1
C(42)	-1005(5)	1529(5)	670(2)	26(2)	1
C(43)	-1378(6)	1292(5)	414(3)	34(3)	1
C(44)	-1081(7)	1400(6)	143(3)	43(3)	1
C(45)	-410(7)	1737(6)	120(3)	47(3)	1
C(46)	-30(6)	1988(6)	372(2)	36(3)	1
C(51)	10304(7)	679(7)	398(3)	58(4)	1
C(52)	9623(7)	300(7)	398(3)	58(4)	1
C(61)	2789(7)	6052(7)	1668(3)	62(4)	1
C(71)	6648(6)	2451(5)	268(4)	71(11)	0.433(11)
C(72)	6973(8)	2401(7)	22(3)	75(11)	0.433(11)
C(73)	7596(8)	2488(7)	52(3)	36(7)	0.433(11)
C(74)	7896(5)	2625(5)	327(3)	55(9)	0.433(11)
C(75)	7572(3)	2675(3)	573(3)	69(10)	0.433(11)
C(76)	6948(3)	2588(3)	544(3)	75(11)	0.433(11)
C(81)	6580(1)	2705(1)	901(4)	25(6)	0.027(12)
C(82)	7212(1)	3253(1)	892(4)	25(6)	0.027(12)
C(91)	1834(14)	5887(17)	2891(6)	25(6)	0.181(5)
C(92)	1585(11)	5759(16)	2605(7)	25(6)	0.181(5)
C(93)	2008(15)	5971(17)	2365(5)	25(6)	0.181(5)
C(94)	2679(14)	6310(17)	2410(6)	25(6)	0.181(5)
C(95)	2928(11)	6437(17)	2696(7)	25(6)	0.181(5)
C(96)	2506(15)	6226(17)	2936(5)	25(6)	0.181(5)

Table S19. Selected bond lengths [Å] and angles [°] for Complex 9.

Ru-C(1)	1.847(9)	C(1)-Ru-C(8)	98.7(4)
Ru-C(8)	2.084(9)	C(1)-Ru-Cl(1)	102.9(3)
Ru-Cl(1)	2.382(3)	C(8)-Ru-Cl(1)	83.0(3)
Ru-Cl(2)	2.392(2)	C(1)-Ru-Cl(2)	90.0(3)
Ru-P	2.404(3)	C(8)-Ru-Cl(2)	93.3(3)
		Cl(1)-Ru-Cl(2)	166.96(9)
		C(1)-Ru-P	93.5(3)
		C(8)-Ru-P	167.1(3)
		Cl(1)-Ru-P	90.23(9)
		Cl(2)-Ru-P	90.88(9)

Table S20. Bond lengths [Å] and angles [°] for Complex 9.

Ru-C(1)	1.847(9)	C(18)-H(18B)	0.9800
Ru-C(8)	2.084(9)	C(18)-H(18C)	0.9800
Ru-Cl(1)	2.382(3)	C(19)-H(19A)	0.9800
Ru-Cl(2)	2.392(2)	C(19)-H(19B)	0.9800
Ru-P	2.404(3)	C(19)-H(19C)	0.9800
P-C(41)	1.820(10)	C(20)-C(21)	1.374(14)
P-C(35)	1.837(10)	C(20)-C(25)	1.392(14)
P-C(29)	1.839(10)	C(21)-C(22)	1.400(14)
N(1)-C(8)	1.338(11)	C(21)-C(26)	1.510(14)
N(1)-C(11)	1.447(12)	C(22)-C(23)	1.403(15)
N(1)-C(9)	1.483(12)	C(22)-H(22)	0.9500
N(2)-C(8)	1.349(12)	C(23)-C(24)	1.381(15)
N(2)-C(20)	1.441(12)	C(23)-C(27)	1.525(15)
N(2)-C(10)	1.476(12)	C(24)-C(25)	1.393(15)
C(1)-C(2)	1.452(13)	C(24)-H(24)	0.9500
C(1)-H(1)	0.9500	C(25)-C(28)	1.520(15)
C(2)-C(3)	1.395(14)	C(26)-H(26A)	0.9800
C(2)-C(7)	1.404(14)	C(26)-H(26B)	0.9800
C(3)-C(4)	1.395(14)	C(26)-H(26C)	0.9800
C(3)-H(3)	0.9500	C(27)-H(27A)	0.9800
C(4)-C(5)	1.365(16)	C(27)-H(27B)	0.9800
C(4)-H(4)	0.9500	C(27)-H(27C)	0.9800
C(5)-C(6)	1.386(16)	C(28)-H(28A)	0.9800
C(5)-H(5)	0.9500	C(28)-H(28B)	0.9800
C(6)-C(7)	1.371(14)	C(28)-H(28C)	0.9800
C(6)-H(6)	0.9500	C(28)-H(28D)	0.9800
C(7)-H(7)	0.9500	C(28)-H(28E)	0.9800
C(9)-C(10)	1.516(14)	C(28)-H(28F)	0.9800
C(9)-H(9A)	0.9900	C(29)-C(30)	1.395(13)
C(9)-H(9B)	0.9900	C(29)-C(34)	1.392(13)
C(10)-H(10A)	0.9900	C(30)-C(31)	1.387(13)
C(10)-H(10B)	0.9900	C(30)-H(30)	0.9500
C(11)-C(16)	1.400(13)	C(31)-C(32)	1.362(14)
C(11)-C(12)	1.410(13)	C(31)-H(31)	0.9500
C(12)-C(13)	1.392(13)	C(32)-C(33)	1.373(14)
C(12)-C(17)	1.499(14)	C(32)-H(32)	0.9500
C(13)-C(14)	1.379(14)	C(33)-C(34)	1.371(13)
C(13)-H(13)	0.9500	C(33)-H(33)	0.9500
C(14)-C(15)	1.377(14)	C(34)-H(34)	0.9500
C(14)-C(18)	1.498(14)	C(35)-C(40)	1.388(13)
C(15)-C(16)	1.406(14)	C(35)-C(36)	1.410(13)
C(15)-H(15)	0.9500	C(36)-C(37)	1.380(13)
C(16)-C(19)	1.517(13)	C(36)-H(36)	0.9500
C(17)-H(17A)	0.9800	C(37)-C(38)	1.364(14)
C(17)-H(17B)	0.9800	C(37)-H(37)	0.9500
C(17)-H(17C)	0.9800	C(38)-C(39)	1.404(14)
C(17)-H(17D)	0.9800	C(38)-H(38)	0.9500
C(17)-H(17E)	0.9800	C(39)-C(40)	1.377(13)
C(17)-H(17F)	0.9800	C(39)-H(39)	0.9500
C(18)-H(18A)	0.9800	C(40)-H(40)	0.9500

C(41)-C(42)	1.399(13)	C(1)-Ru-Cl(2)	90.0(3)
C(41)-C(46)	1.400(14)	C(8)-Ru-Cl(2)	93.3(3)
C(42)-C(43)	1.392(13)	Cl(1)-Ru-Cl(2)	166.96(9)
C(42)-H(42)	0.9500	C(1)-Ru-P	93.5(3)
C(43)-C(44)	1.372(16)	C(8)-Ru-P	167.1(3)
C(43)-H(43)	0.9500	Cl(1)-Ru-P	90.23(9)
C(44)-C(45)	1.379(16)	Cl(2)-Ru-P	90.88(9)
C(44)-H(44)	0.9500	C(41)-P-C(35)	103.2(4)
C(45)-C(46)	1.390(15)	C(41)-P-C(29)	103.6(4)
C(45)-H(45)	0.9500	C(35)-P-C(29)	103.2(4)
C(46)-H(46)	0.9500	C(41)-P-Ru	116.5(3)
C(51)-C(52)#1	1.385(16)	C(35)-P-Ru	117.7(3)
C(51)-C(52)	1.396(17)	C(29)-P-Ru	111.0(3)
C(51)-H(51)	0.9500	C(8)-N(1)-C(11)	126.3(8)
C(52)-C(51)#2	1.385(16)	C(8)-N(1)-C(9)	113.3(8)
C(52)-H(52)	0.9500	C(11)-N(1)-C(9)	119.9(8)
C(61)-C(61)#3	1.377(13)	C(8)-N(2)-C(20)	126.7(8)
C(61)-C(61)#4	1.377(13)	C(8)-N(2)-C(10)	112.8(8)
C(61)-H(61)	0.9500	C(20)-N(2)-C(10)	118.6(8)
C(71)-C(72)	1.3900	C(2)-C(1)-Ru	135.8(8)
C(71)-C(76)	1.3900	C(2)-C(1)-H(1)	112.1
C(71)-H(71)	0.9500	Ru-C(1)-H(1)	112.1
C(72)-C(73)	1.3900	C(3)-C(2)-C(7)	117.5(10)
C(72)-H(72)	0.9500	C(3)-C(2)-C(1)	125.2(9)
C(73)-C(74)	1.3900	C(7)-C(2)-C(1)	117.4(9)
C(73)-H(73)	0.9500	C(4)-C(3)-C(2)	120.7(10)
C(74)-C(75)	1.3900	C(4)-C(3)-H(3)	119.7
C(74)-H(74)	0.9500	C(2)-C(3)-H(3)	119.7
C(75)-C(76)	1.3900	C(5)-C(4)-C(3)	119.9(11)
C(75)-H(75)	0.9500	C(5)-C(4)-H(4)	120.1
C(76)-H(76)	0.9500	C(3)-C(4)-H(4)	120.1
C(81)-C(82)#5	1.382(2)	C(4)-C(5)-C(6)	121.0(10)
C(81)-C(82)	1.4057	C(4)-C(5)-H(5)	119.5
C(81)-H(81)	0.9500	C(6)-C(5)-H(5)	119.5
C(82)-C(81)#6	1.382(2)	C(7)-C(6)-C(5)	119.0(11)
C(82)-H(82)	0.9500	C(7)-C(6)-H(6)	120.5
C(91)-C(92)	1.3900	C(5)-C(6)-H(6)	120.5
C(91)-C(96)	1.3900	C(6)-C(7)-C(2)	122.0(11)
C(91)-H(91)	0.9500	C(6)-C(7)-H(7)	119.0
C(92)-C(93)	1.3900	C(2)-C(7)-H(7)	119.0
C(92)-H(92)	0.9500	N(1)-C(8)-N(2)	108.1(8)
C(93)-C(94)	1.3900	N(1)-C(8)-Ru	123.3(7)
C(93)-H(93)	0.9500	N(2)-C(8)-Ru	127.4(7)
C(94)-C(95)	1.3900	N(1)-C(9)-C(10)	102.5(8)
C(94)-H(94)	0.9500	N(1)-C(9)-H(9A)	111.3
C(95)-C(96)	1.3900	C(10)-C(9)-H(9A)	111.3
C(95)-H(95)	0.9500	N(1)-C(9)-H(9B)	111.3
C(96)-H(96)	0.9500	C(10)-C(9)-H(9B)	111.3
		H(9A)-C(9)-H(9B)	109.2
C(1)-Ru-C(8)	98.7(4)	N(2)-C(10)-C(9)	103.2(8)
C(1)-Ru-Cl(1)	102.9(3)	N(2)-C(10)-H(10A)	111.1
C(8)-Ru-Cl(1)	83.0(3)	C(9)-C(10)-H(10A)	111.1

N(2)-C(10)-H(10B)	111.1	H(19A)-C(19)-H(19C)	109.5
C(9)-C(10)-H(10B)	111.1	H(19B)-C(19)-H(19C)	109.5
H(10A)-C(10)-H(10B)	109.1	C(21)-C(20)-C(25)	121.8(10)
C(16)-C(11)-C(12)	121.2(9)	C(21)-C(20)-N(2)	118.2(9)
C(16)-C(11)-N(1)	119.5(9)	C(25)-C(20)-N(2)	119.9(10)
C(12)-C(11)-N(1)	119.0(9)	C(20)-C(21)-C(22)	118.6(10)
C(13)-C(12)-C(11)	118.0(9)	C(20)-C(21)-C(26)	122.0(10)
C(13)-C(12)-C(17)	120.3(9)	C(22)-C(21)-C(26)	119.4(10)
C(11)-C(12)-C(17)	121.6(9)	C(21)-C(22)-C(23)	121.3(11)
C(14)-C(13)-C(12)	122.0(10)	C(21)-C(22)-H(22)	119.4
C(14)-C(13)-H(13)	119.0	C(23)-C(22)-H(22)	119.4
C(12)-C(13)-H(13)	119.0	C(24)-C(23)-C(22)	117.9(11)
C(15)-C(14)-C(13)	118.8(10)	C(24)-C(23)-C(27)	121.6(11)
C(15)-C(14)-C(18)	120.1(10)	C(22)-C(23)-C(27)	120.4(12)
C(13)-C(14)-C(18)	121.0(10)	C(23)-C(24)-C(25)	122.1(10)
C(14)-C(15)-C(16)	122.2(10)	C(23)-C(24)-H(24)	119.0
C(14)-C(15)-H(15)	118.9	C(25)-C(24)-H(24)	119.0
C(16)-C(15)-H(15)	118.9	C(24)-C(25)-C(20)	118.2(11)
C(15)-C(16)-C(11)	117.5(9)	C(24)-C(25)-C(28)	120.4(10)
C(15)-C(16)-C(19)	120.7(9)	C(20)-C(25)-C(28)	121.4(10)
C(11)-C(16)-C(19)	121.7(9)	C(21)-C(26)-H(26A)	109.5
C(12)-C(17)-H(17A)	109.5	C(21)-C(26)-H(26B)	109.5
C(12)-C(17)-H(17B)	109.5	H(26A)-C(26)-H(26B)	109.5
H(17A)-C(17)-H(17B)	109.5	C(21)-C(26)-H(26C)	109.5
C(12)-C(17)-H(17C)	109.5	H(26A)-C(26)-H(26C)	109.5
H(17A)-C(17)-H(17C)	109.5	H(26B)-C(26)-H(26C)	109.5
H(17B)-C(17)-H(17C)	109.5	C(23)-C(27)-H(27A)	109.5
C(12)-C(17)-H(17D)	109.5	C(23)-C(27)-H(27B)	109.5
H(17A)-C(17)-H(17D)	141.1	H(27A)-C(27)-H(27B)	109.5
H(17B)-C(17)-H(17D)	56.3	C(23)-C(27)-H(27C)	109.5
H(17C)-C(17)-H(17D)	56.3	H(27A)-C(27)-H(27C)	109.5
C(12)-C(17)-H(17E)	109.5	H(27B)-C(27)-H(27C)	109.5
H(17A)-C(17)-H(17E)	56.3	C(25)-C(28)-H(28A)	109.5
H(17B)-C(17)-H(17E)	141.1	C(25)-C(28)-H(28B)	109.5
H(17C)-C(17)-H(17E)	56.3	H(28A)-C(28)-H(28B)	109.5
H(17D)-C(17)-H(17E)	109.5	C(25)-C(28)-H(28C)	109.5
C(12)-C(17)-H(17F)	109.5	H(28A)-C(28)-H(28C)	109.5
H(17A)-C(17)-H(17F)	56.3	H(28B)-C(28)-H(28C)	109.5
H(17B)-C(17)-H(17F)	56.3	C(25)-C(28)-H(28D)	109.5
H(17C)-C(17)-H(17F)	141.1	H(28A)-C(28)-H(28D)	141.1
H(17D)-C(17)-H(17F)	109.5	H(28B)-C(28)-H(28D)	56.3
H(17E)-C(17)-H(17F)	109.5	H(28C)-C(28)-H(28D)	56.3
C(14)-C(18)-H(18A)	109.5	C(25)-C(28)-H(28E)	109.5
C(14)-C(18)-H(18B)	109.5	H(28A)-C(28)-H(28E)	56.3
H(18A)-C(18)-H(18B)	109.5	H(28B)-C(28)-H(28E)	141.1
C(14)-C(18)-H(18C)	109.5	H(28C)-C(28)-H(28E)	56.3
H(18A)-C(18)-H(18C)	109.5	H(28D)-C(28)-H(28E)	109.5
H(18B)-C(18)-H(18C)	109.5	C(25)-C(28)-H(28F)	109.5
C(16)-C(19)-H(19A)	109.5	H(28A)-C(28)-H(28F)	56.3
C(16)-C(19)-H(19B)	109.5	H(28B)-C(28)-H(28F)	56.3
H(19A)-C(19)-H(19B)	109.5	H(28C)-C(28)-H(28F)	141.1
C(16)-C(19)-H(19C)	109.5	H(28D)-C(28)-H(28F)	109.5

H(28E)-C(28)-H(28F)	109.5	C(45)-C(46)-C(41)	120.6(11)
C(30)-C(29)-C(34)	118.9(9)	C(45)-C(46)-H(46)	119.7
C(30)-C(29)-P	118.3(7)	C(41)-C(46)-H(46)	119.7
C(34)-C(29)-P	122.7(8)	C(52)#1-C(51)-C(52)	119.7(16)
C(29)-C(30)-C(31)	119.5(10)	C(52)#1-C(51)-H(51)	120.2
C(29)-C(30)-H(30)	120.3	C(52)-C(51)-H(51)	120.2
C(31)-C(30)-H(30)	120.3	C(51)#2-C(52)-C(51)	120.3(16)
C(32)-C(31)-C(30)	120.7(10)	C(51)#2-C(52)-H(52)	119.8
C(32)-C(31)-H(31)	119.6	C(51)-C(52)-H(52)	119.8
C(30)-C(31)-H(31)	119.6	C(61)#3-C(61)-C(61)#4	119.99(5)
C(31)-C(32)-C(33)	120.1(10)	C(61)#3-C(61)-H(61)	120.0
C(31)-C(32)-H(32)	119.9	C(61)#4-C(61)-H(61)	120.0
C(33)-C(32)-H(32)	119.9	C(72)-C(71)-C(76)	120.0
C(32)-C(33)-C(34)	120.4(10)	C(72)-C(71)-H(71)	120.0
C(32)-C(33)-H(33)	119.8	C(76)-C(71)-H(71)	120.0
C(34)-C(33)-H(33)	119.8	C(73)-C(72)-C(71)	120.0
C(33)-C(34)-C(29)	120.4(10)	C(73)-C(72)-H(72)	120.0
C(33)-C(34)-H(34)	119.8	C(71)-C(72)-H(72)	120.0
C(29)-C(34)-H(34)	119.8	C(74)-C(73)-C(72)	120.0
C(40)-C(35)-C(36)	118.4(9)	C(74)-C(73)-H(73)	120.0
C(40)-C(35)-P	120.5(7)	C(72)-C(73)-H(73)	120.0
C(36)-C(35)-P	121.2(8)	C(75)-C(74)-C(73)	120.0
C(37)-C(36)-C(35)	120.8(10)	C(75)-C(74)-H(74)	120.0
C(37)-C(36)-H(36)	119.6	C(73)-C(74)-H(74)	120.0
C(35)-C(36)-H(36)	119.6	C(74)-C(75)-C(76)	120.0
C(38)-C(37)-C(36)	120.4(10)	C(74)-C(75)-H(75)	120.0
C(38)-C(37)-H(37)	119.8	C(76)-C(75)-H(75)	120.0
C(36)-C(37)-H(37)	119.8	C(75)-C(76)-C(71)	120.0
C(37)-C(38)-C(39)	119.4(10)	C(75)-C(76)-H(76)	120.0
C(37)-C(38)-H(38)	120.3	C(71)-C(76)-H(76)	120.0
C(39)-C(38)-H(38)	120.3	C(82)#5-C(81)-C(82)	119.88(17)
C(40)-C(39)-C(38)	120.7(10)	C(82)#5-C(81)-H(81)	120.1
C(40)-C(39)-H(39)	119.6	C(82)-C(81)-H(81)	120.1
C(38)-C(39)-H(39)	119.6	C(81)#6-C(82)-C(81)	119.94(17)
C(39)-C(40)-C(35)	120.3(10)	C(81)#6-C(82)-H(82)	120.0
C(39)-C(40)-H(40)	119.9	C(81)-C(82)-H(82)	120.0
C(35)-C(40)-H(40)	119.9	C(92)-C(91)-C(96)	120.0
C(42)-C(41)-C(46)	118.7(10)	C(92)-C(91)-H(91)	120.0
C(42)-C(41)-P	120.6(8)	C(96)-C(91)-H(91)	120.0
C(46)-C(41)-P	120.3(8)	C(93)-C(92)-C(91)	120.0
C(43)-C(42)-C(41)	120.0(10)	C(93)-C(92)-H(92)	120.0
C(43)-C(42)-H(42)	120.0	C(91)-C(92)-H(92)	120.0
C(41)-C(42)-H(42)	120.0	C(92)-C(93)-C(94)	120.0
C(44)-C(43)-C(42)	120.4(11)	C(92)-C(93)-H(93)	120.0
C(44)-C(43)-H(43)	119.8	C(94)-C(93)-H(93)	120.0
C(42)-C(43)-H(43)	119.8	C(95)-C(94)-C(93)	120.0
C(43)-C(44)-C(45)	120.6(11)	C(95)-C(94)-H(94)	120.0
C(43)-C(44)-H(44)	119.7	C(93)-C(94)-H(94)	120.0
C(45)-C(44)-H(44)	119.7	C(94)-C(95)-C(96)	120.0
C(44)-C(45)-C(46)	119.7(11)	C(94)-C(95)-H(95)	120.0
C(44)-C(45)-H(45)	120.2	C(96)-C(95)-H(95)	120.0
C(46)-C(45)-H(45)	120.2	C(95)-C(96)-C(91)	120.0

C(95)-C(96)-H(96)	120.0	C(91)-C(96)-H(96)	120.0

Symmetry transformations used to generate equivalent atoms:
#1 -x+y+2,-x+1,z #2 -y+1,x-y-1,z #3 x-y+2/3,x+1/3,-z+1/3
#4 y-1/3,-x+y+1/3,-z+1/3 #5 -x+y+1,-x+1,z #6 -y+1,x-y,z

Table S21. Anisotropic displacement parameters ($Å^2 x 10^4$) for Complex 9. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ru	188(5)	179(5)	210(4)	6(4)	7(4)	106(4)
Cl(1)	201(13)	244(14)	367(16)	-53(12)	1(11)	109(11)
Cl(2)	233(14)	307(15)	252(14)	-23(11)	-41(11)	146(12)
P	194(14)	202(14)	217(14)	15(11)	23(11)	119(12)
N(1)	250(50)	230(50)	230(50)	-30(40)	-30(40)	150(40)
N(2)	380(50)	240(50)	240(50)	-40(40)	-60(40)	220(40)
C(1)	260(60)	190(50)	240(60)	-10(40)	0(40)	150(50)
C(2)	340(60)	210(60)	250(60)	10(50)	-20(50)	180(50)
C(3)	400(70)	230(60)	340(70)	70(50)	-30(50)	150(60)
C(4)	490(80)	300(70)	340(70)	-10(60)	-140(60)	150(60)
C(5)	760(100)	440(80)	180(60)	-10(60)	-80(70)	330(80)
C(6)	520(80)	410(80)	260(70)	20(60)	60(60)	170(70)
C(7)	350(70)	350(70)	260(60)	10(50)	0(50)	140(60)
C(8)	200(50)	170(50)	210(60)	-60(40)	-70(40)	70(40)
C(9)	360(70)	350(70)	310(60)	-90(50)	-30(50)	260(60)
C(10)	510(80)	390(70)	260(60)	-50(50)	-40(50)	350(60)
C(11)	250(60)	270(60)	180(50)	-20(40)	30(40)	170(50)
C(12)	230(60)	360(70)	230(60)	-20(50)	60(50)	190(50)
C(13)	270(60)	450(70)	220(60)	0(50)	10(50)	240(60)
C(14)	350(70)	430(70)	230(60)	90(50)	110(50)	300(60)
C(15)	340(70)	260(60)	310(60)	60(50)	140(50)	180(50)
C(16)	230(60)	280(60)	240(60)	-30(50)	60(50)	140(50)
C(17)	200(60)	350(70)	280(60)	-60(50)	-30(50)	100(50)
C(18)	620(90)	530(80)	260(70)	70(60)	100(60)	390(70)
C(19)	230(60)	340(70)	430(70)	-50(50)	0(50)	130(50)
C(20)	420(70)	220(60)	230(60)	-20(50)	-30(50)	220(60)
C(21)	470(70)	220(60)	270(60)	-30(50)	-40(50)	210(60)
C(22)	520(80)	250(60)	400(70)	-10(50)	-30(60)	190(60)
C(23)	640(90)	330(70)	310(70)	30(50)	10(60)	280(70)
C(24)	570(80)	370(70)	230(60)	-40(50)	-120(60)	310(70)
C(25)	450(70)	260(60)	310(70)	-70(50)	-90(50)	250(60)
C(26)	420(70)	270(60)	340(70)	20(50)	-50(60)	150(60)
C(27)	700(100)	590(90)	320(70)	70(70)	-20(70)	250(80)
C(28)	540(80)	360(70)	360(70)	-40(60)	-120(60)	310(70)
C(29)	160(50)	220(50)	240(60)	20(40)	30(40)	120(40)
C(30)	210(60)	270(60)	300(60)	30(50)	0(50)	150(50)
C(31)	320(60)	400(70)	240(60)	60(50)	0(50)	220(60)
C(32)	260(60)	300(60)	380(70)	140(50)	30(50)	160(50)
C(33)	210(60)	210(60)	400(70)	40(50)	20(50)	120(50)
C(34)	200(50)	240(60)	310(60)	-10(50)	0(50)	140(50)
C(35)	210(50)	310(60)	180(50)	-20(40)	0(40)	160(50)
C(36)	260(60)	260(60)	370(70)	20(50)	70(50)	140(50)
C(37)	300(60)	340(70)	390(70)	0(50)	60(50)	210(60)
C(38)	220(60)	400(70)	330(70)	-40(50)	40(50)	170(60)
C(39)	280(60)	340(70)	320(70)	0(50)	40(50)	100(50)

C(40)	230(60)	270(60)	300(60)	20(50)	60(50)	150(50)
C(41)	310(60)	230(60)	220(60)	-20(40)	-20(50)	190(50)
C(42)	320(60)	170(50)	310(60)	10(50)	-30(50)	140(50)
C(43)	360(70)	180(60)	460(80)	-60(50)	-150(60)	120(50)
C(44)	650(90)	350(70)	320(70)	-130(60)	-220(70)	270(70)
C(45)	650(100)	570(90)	270(70)	-60(60)	-20(60)	360(80)
C(46)	410(70)	440(70)	300(70)	10(60)	0(60)	260(60)

Table S22. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for Complex 9.

	x	y	z	U_{iso}
H(1)	854	4112	856	26
H(3)	-642	2900	507	39
H(4)	-816	2861	-4	48
H(5)	13	3572	-313	53
H(6)	1032	4334	-122	51
H(7)	1205	4386	383	40
H(9A)	-401	4470	1905	36
H(9B)	-1104	3938	1774	36
H(10A)	-913	4562	1375	40
H(10B)	-199	5080	1499	40
H(13)	731	3405	2361	34
H(15)	-1089	1955	2196	35
H(17A)	1118	4457	2166	44
H(17B)	637	4609	1977	44
H(17C)	1071	4355	1815	44
H(17D)	766	4490	1806	44
H(17E)	1247	4338	1995	44
H(17F)	814	4593	2157	44
H(18A)	335	2447	2634	64
H(18B)	-156	1802	2454	64
H(18C)	-434	2096	2696	64
H(19A)	-1456	2823	1641	51
H(19B)	-1811	2441	1937	51
H(19C)	-1617	2086	1688	51
H(22)	1523	5858	756	47
H(24)	-183	4955	311	43
H(26A)	874	4995	1437	53
H(26B)	1344	5741	1344	53
H(26C)	1511	5192	1242	53
H(27A)	761	5707	45	85
H(27B)	1410	5713	152	85
H(27C)	1285	6296	244	85
H(28A)	-1115	4022	514	57
H(28B)	-1230	4306	814	57
H(28C)	-1059	3731	825	57
H(28D)	-1154	4018	922	57
H(28E)	-1039	3733	621	57
H(28F)	-1210	4308	610	57
H(30)	127	2291	1605	30
H(31)	-151	1498	1971	36
H(32)	-538	421	1845	37
H(33)	-670	112	1352	32
H(34)	-421	879	983	28
H(36)	816	1532	970	35
H(37)	1842	1713	837	39
H(38)	2638	2731	672	37

H(39)	2394	3578	628	40
H(40)	1369	3405	756	30
H(42)	-1212	1445	857	31
H(43)	-1841	1055	427	41
H(44)	-1341	1240	-30	52
H(45)	-208	1797	-68	56
H(46)	432	2229	356	44
H(51)	10510	1142	396	70
H(52)	9366	506	400	70
H(61)	2414	5628	1671	75
H(71)	6222	2392	248	85
H(72)	6768	2307	-166	90
H(73)	7818	2453	-116	44
H(74)	8322	2684	348	66
H(75)	7776	2769	762	83
H(76)	6726	2623	712	90
H(81)	6522	2279	914	30
H(82)	7581	3196	879	30
H(91)	1545	5742	3056	30
H(92)	1126	5528	2574	30
H(93)	1837	5884	2169	30
H(94)	2968	6454	2246	30
H(95)	3387	6669	2727	30
H(96)	2676	6313	3132	30

Table S23. Crystal Data and Structure Refinement for Complexes 2, 7 and 9.

Compound	**2**	**7**	**9**
formula	$C_{54.50}H_{77}Cl_2N_2PRu$	$C_{49}H_{47}Cl_5N_2PRu$	$C_{52.74}H_{53.74}Cl_2N_2PRu$
	[$C_{46}H_{65}Cl_2N_2PRu$ · C_6H_6 · ½(C_5H_{12})]	[$C_{46}H_{44}Cl_5N_2PRu$ · ½(C_6H_6)]	[$C_{46}H_{47}Cl_2N_2PRu$ · 1.12(C_6H_6)]
formula weight	963.17 [836.97, 78.11, ½(72.15)]	973.23 [934.18, ½(78.11)]	918.59 [830.84, 1.12(78.11)]
crystal system	monoclinic	monoclinic	rhombohedral
space group	$P\,2_1/n$ (# 14)	$P\,2_1/c$ (# 14)	$R\,\bar{3}$ (# 148)
a, Å	12.2949(7)	12.9550(7)	23.6408(7)
b, Å	14.9666(8)	13.7527(7)	23.6408(7)
c, Å	27.1432(15)	25.7007(13)	45.2398(19)
α, °	90	90	90
β, °	97.601(1)	101.754(1)	90
γ, °	90	90	120
volume, $Å^3$	4950.8(5)	4483.0(4)	21896.5(13)
Z	4	4	18
ρ_{calc}, g/cm^3	1.292	1.442	1.258
μ, mm^{-1}	0.49	0.72	0.50
$T_{max,min}$	0.909, 0.863	0.949, 0.819	0.947, 0.881
F_{000}	2044	1996	8622
crystal shape	block	fragment	plate
crystal color	burgundy	dark brown	pale brown
crystal size, mm	0.21 x 0.26 x 0.30	0.07 x 0.18 x 0.29	0.11 x 0.25 x 0.26
T, K	98	98	98
θ range, °	1.5, 28.5	1.6, 28.5	1.3, 28.8
h,k,l limits	-16, 16; -19, 19; -34, 34	-17, 17; -18, 18; -34, 34	-30, 31; -30, 30; -60, 58
data measured	87057	102600	110902
unique data	11892	10763	11939

R_{int}	0.047	0.097	0.074
data, $F_O>4\sigma(F_O)$	10104	7096	8768
parameters / restraints	751 / 0	529 / 0	505 / 7
R1[a],wR2[b]; all data	0.048, 0.078	0.097, 0.084	0.081, 0.138
R1[a],wR2[b]; $F_O>4\sigma(F_O)$	0.037, 0.076	0.055, 0.080	0.056, 0.136
GOF[c] on F^2	2.66	1.87	3.79
$\Delta\rho_{max,min}$, e·Å^{-3}	0.99, -1.03	2.17, -1.35	2.08, -0.83

All data were collected on a Bruker SMART 1000 ccd with graphite monochromated MoKα radiation (λ=0.71073 Å).

[a] $R1 = \Sigma||F_o|-|^cF_c|| / \Sigma|F_o|$ [b] $wR2 = \{ \Sigma[w(F_o^2-F_c^2)^2] / \Sigma[w(F_o^2)^2] \}^{1/2}$ [c] $GOF = S = \{ \Sigma[w(F_o^2-F_c^2)^2] / (n-p) \}^{1/2}$